NPL Report

ZINC 3.2 (Finite element code) User Manual

John Blackburn

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ABSTRACT

This document describes the operation of ZINC, version 3.2. ZINC is a program to solve (non-linear) multiphysics problems using the finite element method. It can be used to model almost any physics system.

NPL Report

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We gratefully acknowledge the financial support of the UK Department for Innovation, Universities and Skills (National Measurement System Directorate)

Approved on behalf of the Managing Director, NPL by Markys Cain,
Knowledge leader for the Materials Team

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Chapter 1

Introduction

ZINC is a finite element code capable of solving a wide range of physics and multiphysics problems. ZINC can solve pretty much any physics based problems which can be expressed as second order partial differential equations. Examples of physics systems which can be solved include: electrostatics, magnetics, elastic theory, thermal fluctuation, diffusion etc. Further, any *combination* of these physics theories can also be solved as well. ZINC has been successfully used to solve piezoelectric (elastic+electric), multiferroic (elastic+electric+magnetic) and fuel cells (multiple component diffusion+pressure variation). A near-infinity of other systems could also be solved including all the most common scenarios in electromangetics, mechanics, thermodynamics, fluid flow, diffusion and so on. The reason for ZINC's generality is that it is fundamentally a *mathematical* rather than physics program. ZINC solves equations and it is up to the user to tune those equations to correspond to the needed physics system. This requires a certain mathematical skill and familiarity with the problem in hand. However, we believe that no FE code is a substitute for such knowledge: computer modelling is a highly skilled process and cannot be done without skilled human input. We'll see fully automated modelling the day we have lawyer-less courtrooms and doctor-less hospitals! Nonetheless, the level of skill required to use ZINC is not enormously high. Anyone with a physics, maths or engineering degree should have no difficulty following the step-by-step instructions in this manual. If users don't wish to set up their own problems, they can come to NPL for help. Once a set of input files has been prepared, it is easy to adapt it to, say, change material properties or geometry without needing to adjust the detailed physics. Several examples of common physics systems are supplied in the supplied Tutorial Manual and it should be easy to adapt these for many "bread and butter" problems. The beauty of ZINC is that it can solve these familiar problems at full speed while at the same time allowing the simulation of completely new or esoteric equations, which might never have been written down before, let alone solved!

However, before we get too carried away, we should admit that ZINC, in common with other general purpose FE packages, cannot necessarily solve *any* problem input to it. Some problems will turn out to self-contradictory, a fact which is not always obvious when the equations are written on paper. Other systems may be unstable giving a very poorly conditioned matrix and needing special techniques to solve. ZINC comes with several built-in solvers, but users having particular problems should approach NPL for advice. In some cases, problem-specific solution techniques may be needed which NPL can possibly provide. We would like to emphasise that this limitation is not specific to ZINC but is a necessary feature of all general-purpose FE programs. For example, we have tested ZINC extensively against Comsol. When the equations

were well-formed, ZINC and Comsol both solved the problem and gave the same answer. When the equation were not well formed, both solvers failed to converge and terminated with errors. In general, the only way to see if a set of equations will solve nicely is to try solving them.

1.1 Comparison to other general purpose FE programs

As mentioned we have tested ZINC against Comsol quite extensively. In Comsol, equations can be set up in the so-called "coefficient mode", the "strong mode" and the "weak mode". ZINC's operation mirrors Comsol's *coefficient mode*. That is the coefficients in a set of partial differential equations are set to specify the required mathematical system. A simulation run in ZINC can therefore be easily transfered to Comsol and vice versa. However, we have not implemented the "strong" and "weak" formulations because most physics problems are naturally formulated as differential equations. (It has been said that physics is the simply the study of differential equations). The "strong" and "weak" formulations of Comsol are an alternative way of writing the laws of physics which, however, do not appear naturally in most areas of physics, but involve reformulating problems using advanced mathematical techniques. Above we've said that it takes first year undergraduate skills to form the ZINC (and Comsol coefficient mode) equations, but these weak and strong forms are more complex requiring at least PhD in mathematics or theoretical physics. Given that most physical laws are not written in this way, the "strong" and "weak" forms seem both confusing and unnecessary.

However, many users of Comsol never come across these core formulations but are instead encouraged to "combine" areas of physics to get the system they need. For example a piezo-electric problem, you would combine the "elastic" module with the "electrostatic" module. We strongly believe that this "paint by numbers" approach to physics is extremely dangerous and the user is almost certain to end up simulating something different from what they intended. This method is therefore not supported in ZINC.

Another general purpose FE package we have some experience of is OpenFOAM. Whereas Comsol is very much a point-and-click style program, requiring the user to enter data in a large number of dialog boxes, openFOAM takes the opposite approach, requiring the user to (re)write large portions of code and recompile openFOAM each time a new physics system is attempted (specifically, the user rewrites the "main loop" of the code and calls a large number of built in functions, the operation of which the user must learn in detail). This provides enormous flexibility in that the user can alter the fundamental operation of OpenFOAM, but it also makes it very difficult for people to use the package without specialist help. To use openFOAM you need, in addition to maths and physics knowledge, considerable understanding of C++ (the language openFOAM is written in) and you must also study the internal structure of the openFOAM source code in detail. We can see the advantages that openFOAM has in terms of flexibility but we think that users should not need to be grandmasters of a particular programming language to use an FE package. Also the user should not be exposed so much to the internal workings of the code as they are in OpenFOAM.

In ZINC, we have therefore taken a middle ground. Most users will never need to write any code to use ZINC. You just set up the coefficients to correspond to the physics/material properties you want. Running a new physics problem just involves altering the input file: no programming needed. To support non-linearity, material properties can be entered as expressions of the variables being solved for. For instance, if you are solving a dielctric problem you can

In Fortran:

```
function cfun(string,x,y,z,ur,dur,nvar,istep)
  character(*) string
  double precision x,y,z,ur(1),dur(1,3)
  integer nvar

  if (string.eq.'$permittivity') Cfun=1+2*ur(1)    ! ie, permttivity = 1+2*V
end function cfun
```

In C:

```
double cfun(char *label, double *x, double *y, double *z,
     double ur[3], double dur[3][1], int *nvar, int *istep, int length)
{
  if (equal(label,length,"$permittivity"))
     return 1+2*ur[0];                          // ie, permittivity = 1+2*V
}
```

Figure 1.1: Example of functions used in ZINC for non-linear simulation. Fortran and C forms are showed but any language capable of producing a DLL can be used. Function "equal" is described in Figure 5.2

set the permittivities to be constants like `1.0` or expressions like `1+2*V` (where, for example, V is the electrostatic potential). In the latter case the problem would be non-linear since the permittivities depend on the potentials being solved for. Arbitrary expressions may be entered depending on the solution variables (and their derivatives) and/or space position `(x,y,z)`. For conveniance the user can also refer to constants (in the `.con` file, see Section 5.4) which can be altered between simulations. Thus we can change the shape of the system or its material properties without going into details within the main "physics" input file (`.zin`).

However, sometimes a simple expression like `1+2*V` will not be sufficient: it may is necessary to do a complex calculation with loops and branches to discover the material properties. An extreme case might involve running a molecular dynamics code to discover the material property. This code could easily be larger than ZINC itself! ZINC can therefore, optionally, be made to link to arbitrary code. Instead of setting `1+2*V`, the user writes several functions, an example of which is shown in Figure 1.1.

This function (and a few others like it) is *all* that is expected from the user even in this "advanced" method of using ZINC. Note that any programming language can be used provided it can be compiled into a Dynamic Link Library (DLL). Unlike OpenFOAM, ZINC is deliberately language agnostic and never needs to be recompiled. The user simply provides a function (in a DLL) which calculates the needed material property given the point in space `x,y,z` and the solved-for variables (`ur`) and their derivatives (`dur`). The user is *entirely shielded* from the inner working of ZINC, and just needs to fill out a purely mathematical function. Of course instead of the single line `Cfun=1+2*ur(1)`, as above, the user can enter arbitrarily complex code with loops, branches, calls to other functions, read/write from files etc. We believe that this approach is much simpler and more effective than the OpenFOAM technique. Note again that programming

is optional, and only needed for advanced simulations. Full details of user functions accessed by ZINC are given in Section 5.3.

1.2 Zinc operation

With these ideas in mind, let us look at the operation of ZINC, which is shown diagrammatically in Figure 1.2. This looks complex but bear with us! The user can choose any stem name "file" for the simulation. Thus, `file.zin` might become `fuelcellcathode.zin` for example. The `file.zin` file contains all information about the physics of the problem to be solved. `file.con` (optional) contains a list of convenient constants in the simulation which will be referred in `file.zin`. Eg, we can store `eps0=8.854e-12`, the permittivity of free space. The permittivity of a material with rel. permittivity 2 can then be entered as `2*eps0` rather than the more cumbersome `1.778e-11`. `file.dll` contains the above-mentioned non-linear functions (if needed), more details of which are shown in Section 5.5.

Before a geometry can be solved in FE it needs to be broken up into many small shapes called elements through a process known as meshing. ZMESH provides the functionalilty. The user writes `file.min` which specifies the geometry in a simple way. ZMESH then processes this file and outputs `file.mtf` which contains the geometry and position of all the elements.

ZINC then runs and writes an output file `file.zou` containing the solution on each of the FE nodes. This file can be viewed directly using ZMESH but for more advanced views and post processing, the code ZPP is provided. ZPP (ZINC post processor) reads the file `file.zpp`, in which the user specifies a series of linescans and/or plane scans and generates corresponding graphs. The user can plot arbitrary expressions based on the simulation variables and their derivatives. ZPP automatically plots all files on the screen and also creates graph files in the form of Enhanced Metafiles (EMF) or Encapsulated Postscript (EPS) files. EMF files are convenient for Microsoft Office products while EPS is most suitable for LaTeX: both are vector formats.

In order to generate these graphs, ZPP outputs the datafiles `file01.out, file02.out...` etc. These are simply numbered in order created (depending on how many such plots the user has requested). ZPP then calls Gnuplot (using auto-generated command file `file.gnu`) to generate the graphs needed. Since the `*.out` files are still left behind on disk, its easy to recreate the graphs when needed. The user can use Gnuplot to change the symbols, titles and formatting of the graph or to plot several simulation results in one graph. It's easy, for example, to compare simulation results with experimental data. Since the raw data files are always on disk there's never any mystery about where a graph came from. This approach therefore provides good traceability and flexiblity. See the Tutorial Manual, Chapter 1 for more details on advanced graph plotting.

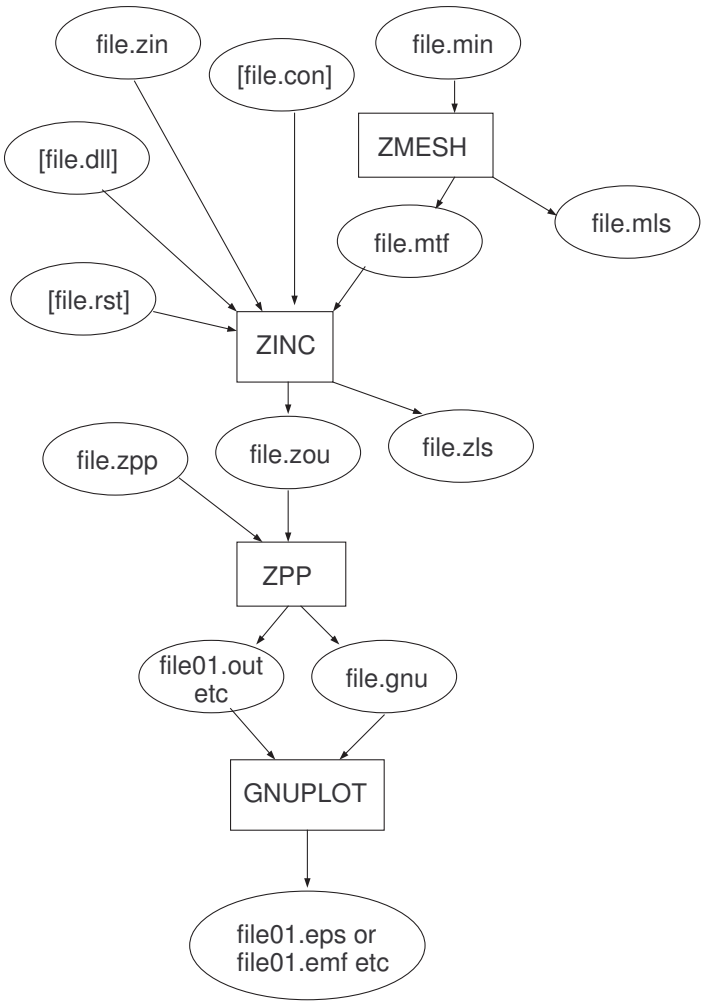


Figure 1.2: The operation of ZINC. Ellipses are files and rectangles are programs. Optional input files are shown in [brackets]. The DLL file can be generated using any programming language

Chapter 2

Installing and running Zinc

ZINC is installed using an automatic installer which will guide you through the process. The three programs, ZMESH, ZINC, ZPP, are available to run from the Start Menu in Windows. The programs can also be invoked from the command line as

```
zmesh filename
zinc filename
zpp filename
```

This latter technique is useful for running ZINC under batch control. ZINC can also be run from external programming systems like Matlab, Python or Excel.

The actual filenames for the ZINC programs are:

zinc.exe Core solver, runs at the command line.

zincwin.exe Windows version of ZINC.

zpp.exe Post processor, runs at the command line.

zppwin.exe Windows version of ZPP.

zmesh.exe Non-interactive mesh generation.

zmeshwin.exe Interactive mesh generation/visualization package.

When ZINC installs, the windows versions of ZMESH, ZINC, and ZPP appear in the Start Menu. The installer adds ZINC's directory to your PATH so that you can conveniently run ZINC from the command prompt. Windows programs like `zincwin.exe` operate by calling their command line equivalents, like `zinc.exe`.

ZINC also comes bundled with Gnuplot. ZPP invokes Gnuplot to generate graphs. Gnuplot is then available for the user to run independently from ZINC. Gnuplot comes with documentation and many tutorial examples. Since ZPP emits text output files as well, these can be plotted using any graph plotter or spreadsheet program. However, we recommend the user of Gnuplot for best speed and quality.

For advanced, non-linear operation, the user will need to prepare DLL files for ZINC to link to. A free compiler like `gcc` or `gfortran` will do (`http://gcc.gnu.org/wiki/GFortran`). See the Tutorial Manual, Chapter 3, for an example of preparing a DLL file to link to ZINC. The user does not need to recompile ZINC.

2.1 Zinc install directory

In the install directory you will find the directory `examples`. This contains several worked examples which are described in the Tutorial Manual. Also there is a `mesh_examples` directory which contains various meshing examples (`.min` files). You should try some of these out in ZMESH.

Other useful files include `nltemplate.f90, nltemplate.c` which contain empty user specified functions for non-linear simulations. If you are running an advanced non-linear simulation, you can create your non-linear functions by copying these templates and filling in the functions provided.

If you are running ZINC from another system like Python or Matlab, it may be preferable to run ZINC and ZPP indirectly using the provided batch files `zincrun, zpprun`. These short batch files simply ensure that the ZINC, ZPP command prompts stay open should an error occur. Otherwise you will not be able to read the error before the box closes. Useage:

```
zincrun file
zpprun file
```

2.2 Uninstalling zinc

Simply use the "Unistall" icon in the Start Menu. If you install a newer version of ZINC, you should uninstall the old version first. Note, everything in the ZINC install directory will be deleted so you *should not store simulation runs in the* ZINC *install directory.*

2.3 Linux and Mac

While ZINC has been written for Windows computers, it should run perfectly on Linux and Mac using the Wine system. Wine comes bundled with most Linux systems and is available for download on Mac. The Wine website contains comprehensive information on running Windows programs with Wine. To install ZINC, you should run the installer executable through Wine. Then run ZMESH, ZINC and ZPP through Wine.

One issue we've noticed on Linux: it's better to install ZINC in a directory without spaces in its path, i.e., *not* in the default `c:\program files\zinc` directory. Similarly the directory where you store your actual simulations should probably be free of spaces.

2.4 Zinc Memory requirements

Most of ZINC's memory requirement is due to storing the matrix Q. This is stored in sparse format in `Qval(ip), iQ(ip), jQ(ip), ip=1,...,lenQ` where `lenQ=nnod*nvar`^{2}`*27`. Here, `nnod, nvar` are the total number of nodes and number of variables respectively. ZINC uses 8 byte real numbers (double precision) and 4 byte integers. Therefore each entry in Q uses 8+4+4=16 bytes and the memory requirement is about `nnod*nvar`^{2}`*27*16` bytes.

Chapter 3

Meshing with Zmesh

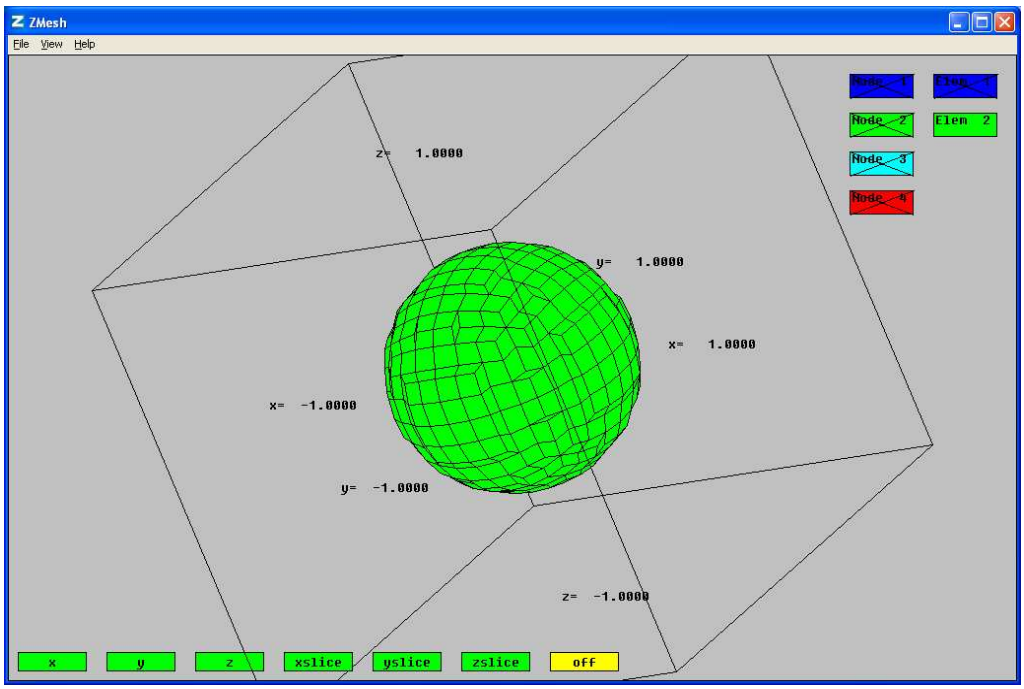
Before we can simulate a problem in ZINC, the geometry must first be meshed. This is the process of decomposing the required geometry into small *elements*. ZINC requires that the geometry be meshed into *hexahedral elements* and this may be accomplished by using the included program ZMESH. A hexahedron is a six sided solid figures resembling a squashed cube. Cuboids are special cases of hexahedrons: if the geometry is a laminar system, for example, it may be sufficient to use cuboid hexahedrons. In general, however, ZMESH will distort the hexahedrons so as to conform to surfaces in the geometry specified. ZMESH works by reading in the geometry specification from file `file.min` and writing out `file.mtf` which contains the shape and position of each element. `file.mtf` is just a text file, whose format is described in Section B, so you can write your own program to do the meshing if you want. This may be useful in cases where the geometry consists of irregular shapes. For example, we had a project to model the stress/strain of ferroelectric domains. We wrote a program to convert the domain map output by a microscopic imaging device into the corresponding `file.mtf`. ZMESH would not have been helpful in this case, since the shapes are irregular and better represented as a "map" rather than a series of primitive shapes like spheres and boxes.

ZMESHuses the same geometry specification format as MetaMesh, a commercial meshing program available from Field Precision[1]. As such, MetaMesh can be used in place of ZMESH if required. Metamesh has many more features than ZMESH including a CAD front end and the ability to read stereo lithography and popular CAD files for geometry specification. Although more basic, ZMESH will do the job in most systems and at least it's free! The user may want to try using ZMESH first, to see whether the ZINC package as a whole is suitable to their needs. Then, if more sophisticated geometries are needed, the user can opt to purchase MetaMesh directly from the Field Precision website.

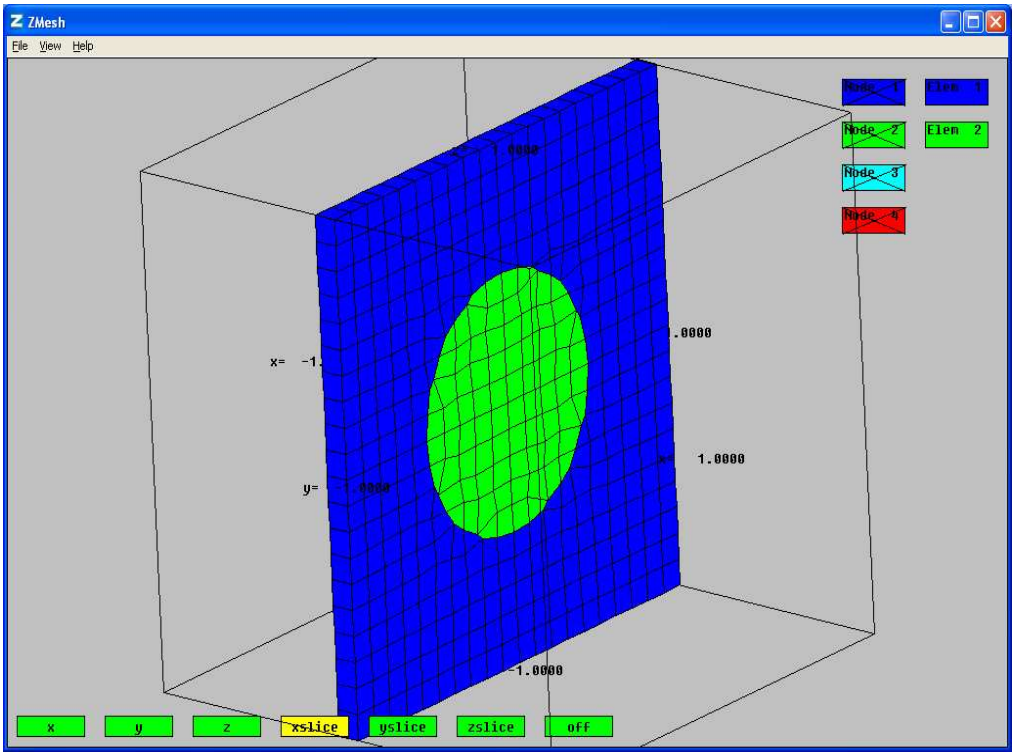
3.1 The Zmesh program

Zmesh is an interactive program as shown in Figure 3.1. The user first prepares an input file, `file.min` which contains all the geometry details, Section 3.2. He then uses the `File > Open MIN` command to read this file. At this point the file can be examined using `File > View MIN`. If all is well, the file can be processed using `File > Process`. A meshed geometry is then created and is saved automatically as `file.mtf`. This geometry appears on screen and can be rotated

[1] www.fieldp.com



(a) Zmesh view with region 1 turned off to expose region 2



(b) Showing an "xslice" through the structure

Figure 3.1: Zmesh: a program for meshing arbitrary structures.

by dragging on screen (the arrow keys can also be used). Various viewing options also exist as described below. A pre-existing mesh file `file.mtf` can be read using `File > open MTF`

If you have already run a ZINC simulation, you can view the result using `File > open ZOU`. This shows a colour-coded view of the data with a colour bar (on the left) indicating value variables. You can cycle through the variables using the "¡" and "¿" buttons. This feature is intended to give a basic look at the raw data solved by the simulation. For post processing, linescans and surface plots (i.e. more quantitative information) use ZPP.

3.1.1 File menu

Open MIN read geometry input file.

Open MTF read pre-processed mesh definition file.

Open ZOU View a solution file. Shows a basic view of the data. For more advanced views and post processing, use ZPP.

View MIN Show input file on screen. Note that this file cannot be edited. The user should use a text editor to edit the file. Notepad will do but a programming text editor may be preferable. We use Emacs, a free text editor with many advanced features. For complex geometries it may be necessary to generate `file.min` using a computer program.

Process Process the currently loaded MIN file.

Exit Terminate the program

3.1.2 View Menu

Bounding box Brings up a dialog allowing user to select a rectangular section of the simulation volume to display. User selects minimum and maximum `i,j,k` values (indexing system for elements). The maximum extents allowed are shown to the right of the dialog. Click "All" to set the maximum extents and show the whole system. Click "one" to select only one element which is taken to be that specified by `imin, jmin, kmin`

Export View Allows you to export the current view as an Enhanced Metafile (EMF).

Copy View Copies the current view to the clipboard.

3.1.3 On screen controls

Drag the on screen objects with the mouse to rotate (or use arrow keys). Zoom in/out using keys "A" and "Z". Rotate in the plane using keys "N" and "M". Shift the view around by holding "Shift" and dragging with the mouse.

A legend for the region numbers are listed on the right of the screen. Left click to toggle a region on or off. (when a region is off a cross appears in the box). For example, in Figure 3.1(a), region 1 has been switched off allowing easier viewing of region 2 (a sphere in this case). When viewing a simultion result file (ZOU file), these buttons have three states: on, DATA, off. The DATA state shows colour coded data for the given region with a colour legend on the left.

Right clicking on a region in the legend brings up a colour dialog box which allows the user to change the colour for the indicated region number.

The buttons along the bottom are as follows

x,y,z View along the x, y or z axes.

xslice, yslice, zslice View a slice through the system (ie a single plane of elements), for example as shown in Figure 3.1(b). You can change which slice is displayed using the up and down arrows on the keyboard.

off Switch off slices so that the whole system is displayed.

3.1.4 Output window

ZMESH gives various notifications to the user in the output window. These include, details of meshing or any errors encountered in the input file.

3.2 Structure of the geometry input file

The mesh input file `file.min` has the form

```
global
   <global commands>
end

part 1
   <part commands>
end

part 2
   <part commands>
end

:

endfile
```

The global commands specifies the *logical mesh* and various global variables which define the quality of the meshing. The part commands define various shapes (spheres, cubes, extrusions etc) that make up the geometry needed. Note that *later parts overlap earlier ones so the order of parts is important.* The logical mesh is illustrated in Figure 3.2: it is a simple cuboid mesh defined by the global commands `xmesh, ymesh, zmesh` as illustrated in that figure. The logical mesh defines the number of elements and nodes (intersection of the lines shown) in the simulation and also the extent of the simulation. In Figure 3.2, for example, the simulation stretches from -0.5 to 0.5 in all directions. Note that the overall simulation area is always cuboid shaped. (However, it is possible to model curved outer boundaries by setting the properties of an outer region to correspond to vacuum). Distance units are not specified at this stage, so the value 0.5 may be metres or angstroms. In ZINC input file `file.zin` it is possible to scale the geometry using a scale factor as required, see Section 5.2.1. The global commands `xmesh` has the form

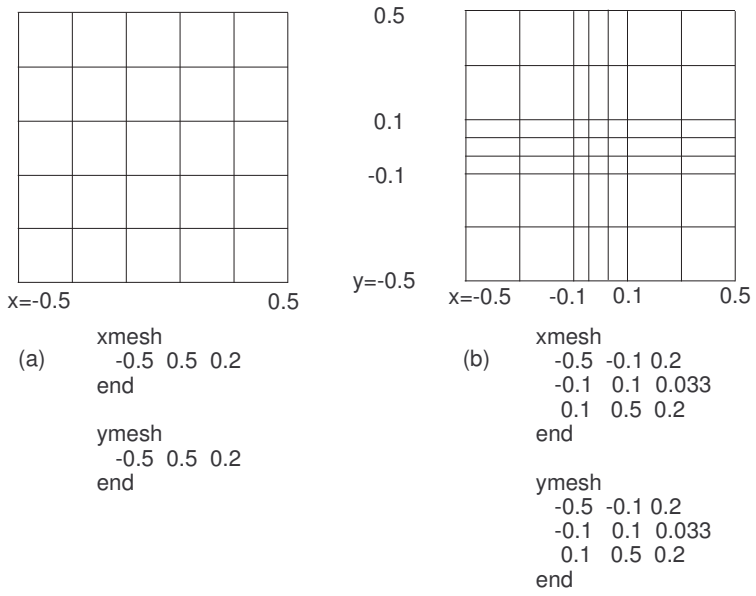


Figure 3.2: Logical mesh formed using the global commands shown. (In the real file a `zmesh` command is also needed. For simplicity, these figures show a 2-D analogy). (a) Single meshing interval with one xmesh and one ymesh command; (b) variable meshing with multiple meshing commands

```
xmesh
  x1  x2 dx1
  x2  x3 dx2
:
end
```

where `[x1,x2]` is a line segment divided into intervals `dx1` wide etc. If `xmesh` contains only one command line, the meshing is uniform across the whole simulation region. If there are multiple lines as in Figure 3.2(b), this allows variable meshing as shown. The commands `ymesh, zmesh` have exactly the same form.

ZMESH then processes the parts one by one as shown in Figure 3.3. In response to the two part commands shown, a sphere is created inside a cube. The cube is specified first and covers the whole simulation region. Then, the sphere is specified which is inserted into the cube (ie the cube is overwritten showing the importance of parts order in the file). Notice that the cube is designated "region 1" and the sphere as "region 2". These region numbers will later be linked to material properties in `file.zin`. Figure 3.3(a) shows what happens in response to the part 2 command. ZMESH identifies the elements whose centroids are inside the sphere specified and sets the elements as region 2. In response to the `surface` command in the part 2 'block', ZMESH then moves nodes so that they lie on the sphere creating a shape which more closely conforms to the sphere. Without the surface command, the elements would remain cuboid and the "sphere" would have the blocky, "staircase" appearance shown in Figure 3.3(a). The final appearance and region number of each element is shown in Figure 3.3(b). (Note that the picture shows an inverted elemnent which would actually be fixed by ZMESH. An inverted element has

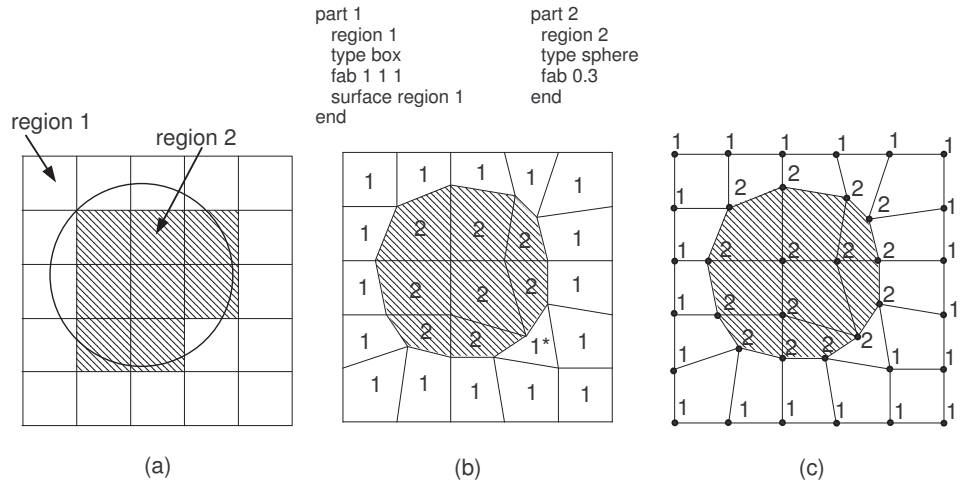


Figure 3.3: Meshing of two parts using the commands shown. The second part (sphere) is inserted into the initial box part. (a) Identification of element region numbers in original logical mesh; (b) nodes are moved onto surface between the two regions. Element region numbers shown. Note that the element marked (*) is not acceptable since it is inverted (see text). In practice, ZMESH avoids inverted elements or at least gives a warning; (c) Final node region numbers

a Jacobian which changes sign across the element preventing the code from integrating correctly over the element (See Theoretical Manual). ZMESH determines whether elements are inverted by calculating the Jacobian. If it is inverted ZMESH relaxes the lattice to attempt to fix the element even if that means having a less conforming mesh. A chevron shaped element is inverted)

Nodes are also given "region numbers" as shown in Figure 3.3(c). This is in order to specify Dirichlet boundary conditions Section 5.2.2 whereby field values are specified on particular nodes. For example, in an electrostatic problem we could designate region 2 nodes as having a fixed potential which would make the sphere into a perfectly conducting object. The default region numbering of nodes – in this example – is shown in Figure 3.3(c): all nodes surrounding an element are given the same region number as that element. Thus, after processing part 1, all nodes are designated region 1. After processing part 2, the elements within the sphere are renumberd region 2 and their surrounding nodes are renumbered region 2 also. In particular the nodes at the interface between the two regions are set to region 2 (since part 2 was processed last). In some cases, it is necessary to override this behaviour and give a different region number to the interface nodes. This can be accomplished by use of the `coat` command as shown in Figure 3.4(a). In this case, while processing part 2, ZMESH gathers all nodes at the interface between this part and region 1 and numbers these as region 6.

Another way to set node region numbers is to use "open parts" as shown in Figure 3.4(b). Here we have used two additional parts (3 and 4). These define surfaces at the top and of the simulation whose nodes are set to region 3 and region 4 respectively. In this example (assuming an electrostatic problem), it would be possible to excite the system by putting 1 V on region 3 nodes (top, Dirichlet boundary) and zero volts on region 4 nodes (bottom, Dirichlet boundary). This would create an electric field on the simulation. In elastic problems, this would correspond

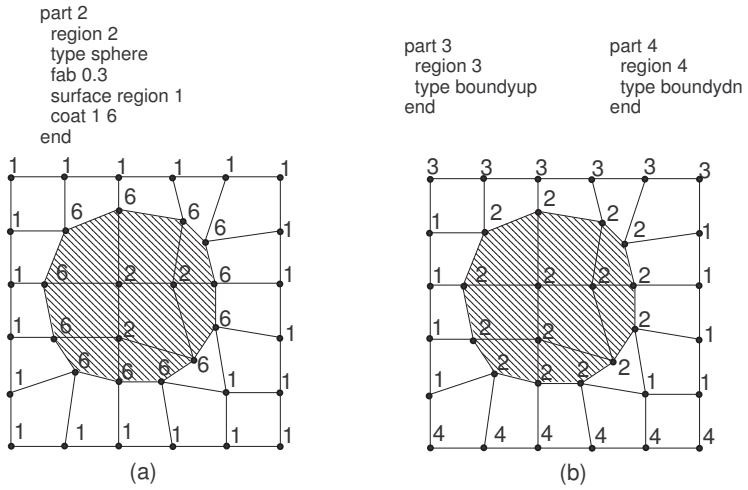


Figure 3.4: (a) Use of the coat command to change the node region numbers at an interface; (b) use of open parts (`boundyup` and `boundydn`) to change the node region numbers

to clamped displacements at the top and bottom of the simulation, and so on.

Figure 3.5 shows the corresponding `file.zin` for Figure 3.4 set up as an electrostatic problem. This file will be described in more detail in Section 5.2 but for now note how region 1 and region 2 elements are given permittivity values of ϵ_0 (permittivity of free space, 8.854×10^{-12} F/m) and $2\epsilon_0$. Also, region 3 and region 4 nodes are set to voltage values 1 V and 0 V respectively. Region 1 and 2 nodes are not set at all, so these nodes (the interior nodes in the problem) are allowed to vary in order to solve the electrostatic equations.

By the end of the part fitting process, all elements and nodes should be given an region number. If this is not the case, ZMESH will report an error. It is common practice for the first part to be a box part which covers the whole simulation area. Other parts are then inserted into this part.

We have so far described most of the part commands: `type, region, fab, surface, coat`. The other two commands are shift and rotate, allowing the part to be shifted and rotated into the required position. Parts are conceptually constructed at the origin $(0, 0, 0)$ with major axes generally along x, y, z. Thus, the "box" part is constructed with principle axes along the x,y,z directions. It is centred at the origin and its extents are given by the 3 numbers following the `fab` (fabricate) command. The meaning of the fab parameters depends on the part and is given in Table 3.1.

The rotation command has the form

```
rotate rx ry rz [string]
```

If string is absent then a rotation is performed about the (global) x-axis, then the y-axis then the z-axis by the angle given, in degrees. If a different order is required, this can be given using the string. Eg using "yzx" would cause rotation to occur about y, then z then x. Since these are Euler angles, *rotation order is important.* Furthermore, *rotation is performed before the object is shifted* irrespective of the order of commands in the part block.

The shift command has the form

```
<global commands>
:
  region 1 elements 3 values C
  V x V x = 8.854e-12
  V y V y = 8.854e-12
  V z V z = 8.854e-12

  region 2 elements 3 values C
  V x V x = 1.7708e-11
  V y V y = 1.7708e-11
  V z V z = 1.7708e-11

  region 3 nodes 1 value
  V=1

  region 4 nodes 1 value
  V=0
```

Figure 3.5: Sample ZINC input file, `file.zin` corresponding to the setup of Figure 3.4(b)

```
  shift x y z
```

and causes the part to be shifted along the displacement specified.

3.3 Neuman Boundaries

So far we have discussed the creation of elements and nodes and their region numbers, which are later associated with volumetric material properties and Neuman boundary conditions respectively. The other boundary condition supported by ZINC is the Neuman boundary condition. Whereas Dirichlet boundaries fix the variables being solved for, eg, voltage, temperature, elastic displacement, Neuman boundaries fix derivatives of these: surface charge, thermal flux, traction respectively. These quantities may be classified as fluxes or applied forces of some kind. Thus fluxes are applied at boundaries which may be internal to the simulation or external. ZMESH does not specify such surfaces explicitly, rather surfaces exist between volumetric regions. For example, the curved surface in Figure 3.4(b) between region 1 and region 2 would be identified $1-2$ giving an extra command in Figure 3.5

```
  surface 1-2  1 value q
     V  V = 1.0

  surface 1-2 1 value g
     V = 2
```

The simulation is conceptually surrounded by regions called “XMAX”, “XMIN”, “YMAX”, “YMIN”, “ZMAX”, “ZMIN”, as shown in Figure 3.6. Thus the red outer edge on the left hand of Figure 3.6 can be designated

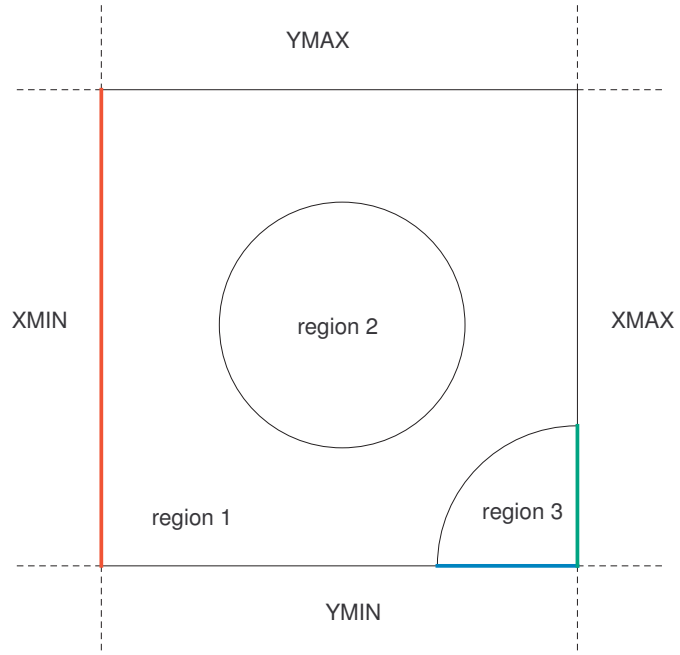


Figure 3.6: Specification of surfaces for Neumann boundary conditions. Surface 1-2 is the circular surface between regions 1 and 2. Surface 1-XMIN is the red surface, surface 3-YMIN is shown blue and surface 3-XMAX is shown green

```
1-XMIN
```

(interface between region 1 and XMIN).

3.4 List of part specification commands

There are seven (7) part specification commands which appear within a part block (`part n...end`). These are: `type, fab, region, surface, coat, rotate, shift`. We have already introduced these commands but now specify them in more detail

type The type of part, see Table 3.1. Single parts are just of the form `type part`. Advanced parts Table 3.3 have the form `type <part> <Vector list> end` with each vector on a separate line, Section 3.8.

fab Fabrication info for the part. This depends on the part in question and is described in Table 3.1, Table 3.2, Table 3.3.

region Elements in this part will be assigned this region number. Nodes around those elements will also be so assigned.

surface This command has the form `surface {region|part} [n] {edge} [tol]`. It causes nodes to be moved towards the surface between the current part and the specified part or region (n). This causes the mesh to conform to the surfaces rather than having a

"staircase" appearance. The `edge` command causes edge fitting to take place also. If present, `tol` determines the speed of relaxation onto the surface. It is a number in the range 0-1. If omitted, the default value is 0.9 is assumed

coat Has the form `coat reg regnew`. Finds all nodes at the interface between the current part and region `reg`. These nodes are then given region number `regnew`.

rotate Has the form `rotate x y z {string}`. By default, rotate part about the x, y and z axes in that order (angles in degrees). If `string` is present, the order of rotation may be altered. Eg `xzy` means rotate about x, then about z, then about y. The order of rotation is important: x,y and z are Euler angles. Rotation is performed before shifting.

shift `shift x y z` shift the part along the vector specified after rotation is complete.

protect Protects node region numbers in current part from being overwritten. This is useful in filled parts whose nodes might be overwritten by open parts. Since open parts are always processed *after* filled parts, it is not possible to simply rearrange the parts order. This only affects node, not elements.

3.5 List of global commands

These commands must appear in the `global` section of the input file.

xmesh, ymesh, zmesh Specified line segments spanning the simulation area in the x direction. This defines the logical mesh. Each line segment is divided into intervals allowing variable meshing. Has the form `xmesh <line segments> end` with each line segment on a separate line of the form `x1 x2 dx`. Commands `ymesh, zmesh` have the same form.

presmooth N Smooths the logical mesh using N smoothing steps. This is only important when variable resolution is used in the logical mesh. Default: no smoothing.

axissmooth dir N Smooths along one direction "dir" only. Dir is either x, y, or z. N is the number of steps. Default: no axis smoothing.

smooth N Smooths the final mesh after part fitting has been accomplished. N steps of relaxation, default 10.

format `Format {ascii|binary}` causes the mesh output file to be text (`file.mtf`) or binary (`file.mdf`) respectively.

3.6 List of basic 3D parts

These parts may be rotated/shifted into position using `rotate` and `shift` commands. They are listed in Table 3.1.

Shape	Fab parameters	Description
`box`	Lx Ly Lz	Centred at origin and extends [-Lx,Lx] along x etc
`sphere`	R	Centred at origin with radius R
`cylinder`	R H	Centred at origin with radius R and extends [-H/2,H/2] along z
`cone`	R H Hz	Truncated cone along z with base at $z = 0$ with radius R. Apex at $z = H$ and truncated at $z = Hz$
`ellipcyl`	Rx Ry H	Cylinder along z with elliptical cross section extending x=[-Rx,Rx], y=[-Ry,Ry]
`ellipsoid`	Rx Ry Rz	Ellipsoid given by $(x/R_x)^2 + (y/R_y)^2 + (z/R_z)^2 = 1$
`torus`	R r	R is major radius and r is minor radius. Plane of the "hole" is normal to z
`helix`	R r H Hw	Circular cross section helix (radius r) which wraps around a z-directed cylinder height H, radius R centred at the origin. Hw is the height along z attained during 1 revolution.
`trapezoid`	LxU LxD Ly Lz	Prism along z with trapezoidal cross section. Full width in x is LxU (top) and LxD (bottom). Full width in y and z given by Ly, Lz

Table 3.1: List of 3-D parts and the meaning of the fab command

3.7 List of open parts

These parts have no volume so elements are not effected. The only result is to change the region numbers of nodes. These parts are 0, 1 or 2-D and may be rotated and shifted into position using `rotate` and `shift` commands. Note that `boundxup` etc do not need fab commands and are unaffected by `rotate` and `shift`. The parts are listed in Table 3.2.

3.8 Advanced parts

ZMESH supports 4 types of advanced parts which allow more general shapes to be created: `extrusion, turning, transition` and `neon`. Whereas the simple parts above have a single line type command (E.g. type sphere), these parts have a multi-line type command of the form,

```
type {extrusion|turning|transition|neon}
   <data lines>
   :
end
```

Apart from this, the part specification is the same and `region, surface, coat, shift, rotate` commands may be used as usual.

3.8.1 Extrusion

An extrusion is a prism shape along the z axis. The cross section is built up using an arbitrary number of line or arc segments which must form a closed 2-d shape in the x-y plane.

The `type` command has the form

Part	fab params	Description
`point`	x y z	Creates a point at (x,y,z)
`boundxup`	(none)	plate comprising the upper x plane of the simulation
`boundxdn`	(none)	plate comprising the lower x plane of the simulation
`boundyup`	(none)	plate comprising the upper y plane of the simulation
`boundydn`	(none)	plate comprising the lower y plane of the simulation
`boundzup`	(none)	plate comprising the upper z plane of the simulation
`boundzdn`	(none)	plate comprising the lower z plane of the simulation
`line`	L	line from (0,0,-L/2) to (0,0,L/2)
`arc`	R θ_{min} θ_{max}	Arc in z=0 plane centred at origin from angle θ_{min} to θ_{min}, radius R. $\theta = 0$ is the x-axis. Angles in degrees.
`circle`	R	open circle centred at origin radius R
`rectangle`	Lx Ly	Open rectangle in z=0 from [-Lx,Lx] in x and [-Ly,Ly] in y
`disk`	R	As circle but filled
`plate`	Lx Ly	As rectangle but filled
`bubble`	R	Spherical surface centred at origin radius R

Table 3.2: List of open parts

```
type extrusion {sidefit}
   Vector 1 {S|SE}
   Vector 2 {S|SE}
   :
end
```

Each vector describes a line or arc in the x-y plane and is of the form

```
{L|A} xstart ystart xend yend {xcentre ycentre}
```

Here, "L" means line and "A" means arc. The `xcentre ycentre` specification is only required for arcs. The line extends from `(xstart,ystart)` to `(xend,yend)` with arc centre (in the case of arcs) at `(xcentre,ycentre)`. Vectors should link to one another in sequence and form a closed loop in the x-y plane. Eg to make a square use

```
type extrusion
 L  0 0   1 0
 L  1 0   1 1
 L  1 1   0 1
 L  0 1   0 0
end
```

To make a circle, we could adapt this to read

```
type extrusion
 A  0 0  1 0  0.5 0.5
 A  1 0  1 1  0.5 0.5
 A  1 1  0 1  0.5 0.5
 A  0 1  0 0  0.5 0.5
end
```

Note that *arc segments may not be more the 90 degrees*. Longer arcs should be divided into smaller ones just as we have done here.

The extrusion fab command takes a single parameter: the length of the extrusion.

```
fab L
```

The extrusion is along the z axis from -L/2 to L/2. The whole extrusion can be rotated and shifted into place in the usual way.

The S and SE commands at the end of each vector determine how surface fitting is done on the extruded surface of the shape. If S is present, the segment is surface fitted. If SE is present edge fitting is done also. Such surface fitting is performed only if a `surface` command appears in the part specification. The top and bottom part of the surface is always fitted if such a surface command is present. To turn off this fitting, use the `sidefit` specifier.

A complete part specification for extrusion looks like, for example,

```
part 1
  region 1
  type extrusion
   L  -1 0   1 0
   A   1 0   0 1   0 0
   A   0 1  -1 0   0 0
  end
  fab 1
  rotate 90 0 0
  shift 1.0 0.0 0.0
end
```

This creates prism of semi-circular cross section, length 1 along the z axis, then rotates it around x so it now points along y. The part is shifted so that its centre is at (1,0,0).

3.8.2 Turning

A turning part is made by constructing a 2-D shape in (r,z) plane then rotating about the z-axis. The type command has exactly the same form as for the extrusion (including the use of lines or arcs and the S/SE commands):

```
type turning {sidefit}
   Vector 1 {S|SE}
   Vector 2 {S|SE}
   :
end
```

The fab command has the form

```
fab angmin angmax
```

where `angmin, angmax` are the minimum and maximum turning angles (about the z axis) in degrees. Use 0 and 360 to produce a full turning. If the angle difference is less than 360 the turning will have "start" and "end" faces which are fitted according to the surface command (unless `sidefit` is specified). The turning may be shifted and rotated in the usual way.

3.8.3 Transition

The transition shape consists of two planar shapes at z=zmin and z=zmax connected together. As we go from zmin to zmax, the shape smoothly "morphs" between the two shapes. The type command has the form

```
type transition {sidefit}
  Vector 1a  Vector 1b  {S}
  Vector 2a  Vector 2b  {S}
  :
end
```

Each vector is of the form

```
xstart ystart xend yend
```

Note that arcs are not allowed so there is no need for the L or A specification. Vector 1a (on the bottom surface) morphs into vector 1b (on the top surface) etc. The "S" parameter, if present, indicates that surface fitting will be done. The fab command has the form

```
fab L
```

The shape then extends along the z axis from z=-L/2 to z=L/2.

3.8.4 Neon

The neon shape is an arbitrary tube of circular cross section. The trajectory of the cross section is given by a series of points:

```
part neon
  x1 y1 z1
  x2 y2 z2
  :
end
```

where (x1,y1,z1) etc are points in 3-D space. The fab command has the form

```
fab r
```

where r is the radius of the tube.

3.8.5 Summary of advanced shapes

The advanced shapes are summarised in Table 3.3.

type	`type` command	`fab`	Description
`extrusion`	type extrusion {sidefit} [Vector list] end	L	extrusion from z=-L/2 to z=L/2
`turning`	type turning {sidefit} [Vector list] end	θ_1 θ_2	turning about z from θ_1 to θ_2 ($^\circ$)
`transition`	type transition {sidefit} [Vector pair list] end	L	transition along z from z=-L/2 to L/2
`neon`	type neon [points list] end	r	Circular tube radius r

Table 3.3: Table of advanced shapes. A Vector has the form `xstart ystart xend yend {xcentre ycentre} {S|SE}`. A Vector pair has the form `xstarta ystarta xstartb ystartb {S}`

Chapter 4

PDE specification

4.1 Mode 1: Static problems

For static systems, ZINC supports the following partial differential equation sets

$$-\nabla \cdot \mathbf{C}\nabla\mathbf{u} + \mathbf{a}\mathbf{u} = \mathbf{f} \tag{4.1}$$

$$\mathbf{n} \cdot \mathbf{C}\nabla\mathbf{u} + q\mathbf{u} = \mathbf{g}, \quad \text{(Neumann)} \tag{4.2}$$

Here $\mathbf{u} = (u_1, u_2, ...)$ where $u_1(x, y, z)$ etc are the independent variables to be solved for. For example u_1 might be electrostatic potential and u_2 temperature (as in the example of Section 4.4). One must set the various components of **C**, **a**, **f**, **q**, **g** so that, when (4.1) is multiplied out, we obtain the needed set of PDEs and boundary conditions. Here, the meaning of grad and div is non-standard. For example, with two variables, we define

$$\nabla\mathbf{u} = (\nabla u_1, \nabla u_2) \tag{4.3}$$

$$\nabla \cdot (\mathbf{a}|\mathbf{b}) = (\nabla \cdot \mathbf{a}, \nabla \cdot \mathbf{b}) \tag{4.4}$$

where $(\mathbf{a}|\mathbf{b})$ is a 6-vector (in 3D space) partitioned into two, 3-vectors. Thus, grad is applied to each element in **u** and div takes groups of three variables and compacts them into one.

These equations can also be written in component form as

$$-\left(C_{ijkl}u_{k,l}\right)_{,j} + a_{ik}u_k = f_i, \quad i = 1, \ldots, N \tag{4.5}$$

$$n_j C_{ijkl}u_{k,l} + q_{ik}u_k = g_i, \quad \text{Neumann} \quad i = 1, \ldots, N \tag{4.6}$$

with summation over repeat indices and N is the number of independent variables to be solved. Here $u_{k,l} = \partial u_k/\partial x_l$ etc. This general PDE specification allows a wide range of systems to be solved including those mentioned in the introduction.

To give an example, in an electrostatics problem, setting C to the permittivity tensor and f to the charge density ρ defines the equation $\nabla \cdot \mathbf{D} = \rho$ and (4.2) (with $q = g = 0$) corresponds to the "natural", Neumann boundary condition $\mathbf{n} \cdot \mathbf{D} = 0$ which is a typical "open boundary" condition for electrostatic problems.

The components of **C**, **a**, **f**, **q**, **g** all vary in space. When the system is meshed, it is divided into a structured mesh of *hexahedral* elements each of which is assigned a *region number*. The mesh is specified in the input file `filename.mtf` (see Section 5.1). The materials file

`filename.zin` specifies **C**, **a**, **f**, **q**, **g** values for each region, thus specifying material properties (such as permittivity in the above example) for each element.

The values of **C**, **a**, **f**, **q**, **g** components may be set to constant values or set to vary depending on the local values of the **u** vector. For example, they might be temperature dependent, in a thermal problem. In this case, the problem becomes non-linear Section 5.5.

Comsol implements a similar set of equations: these are described in Appendix A. A problem set in ZINC may easily be converted to Comsol and vice versa.

4.2 Mode 2: Transient problems

ZINC can solve transient problems of the form

$$\frac{\partial \mathbf{u}}{\partial t} = \nabla \cdot \mathbf{C}\nabla\mathbf{u} - \mathbf{a}\mathbf{u} + \mathbf{f} \tag{4.7}$$

$$\mathbf{n} \cdot \mathbf{C}\nabla\mathbf{u} + \mathbf{q}\mathbf{u} = \mathbf{g}, \quad \text{(Neumann)} \tag{4.8}$$

or, in component format

$$\frac{\partial u_s}{\partial t} = (C_{sjkl}u_{k,l})_{,j} - a_{sk}u_k + f_s, \quad s = 1, 2, .., N \tag{4.9}$$

$$n_j C_{ijkl}u_{k,l} + g_{ik}u_k = g_i, \quad \text{Neumann} \quad i = 1, \ldots, N \tag{4.10}$$

Note that the boundary conditions are the same as in the static case. Again, one can set up either linear or non-linear problems.

4.3 Static and steady state problems

The static mode of ZINC can be made to solve steady state problems as well. Consider the problem where the **u** variables depend on time as

$$u(\mathbf{r}, t) = Re[u_\omega(\mathbf{r}) \exp(j\omega t)] \tag{4.11}$$

In that case we replace $\partial/\partial t$ with $j\omega t$ in the PDEs and the problem again becomes spatial but we are solving for the *phasors* $u_\omega(\mathbf{r})$. These phasors are complex numbers whose modulus indicates time-oscillation amplitude and whose phase gives a phase shift according to (4.11). However, ZINC does not support complex variables so it will be necessary to write $u = u_r + iu_i$ and expand each complex equation in terms of two real equations.

Some harmonic problems give real solutions, for example if the material properties are real (lossless). In that case $u_\omega(\mathbf{r})$ gives amplitudes of oscillation with each point oscillating in phase.

4.4 Example with thermal-electrical coupling

A simple example of how to set the matrices is an electrical conduction/thermal system. In this case we have

$$-\frac{\partial}{\partial x}\left(\sigma_{11}\frac{\partial V}{\partial x}\right) - \frac{\partial}{\partial y}\left(\sigma_{22}\frac{\partial V}{\partial y}\right) - \frac{\partial}{\partial z}\left(\sigma_{33}\frac{\partial V}{\partial z}\right) = 0 \tag{4.12}$$

$$-\frac{\partial}{\partial x}\left(k_{11}\frac{\partial T}{\partial x}\right) - \frac{\partial}{\partial y}\left(k_{22}\frac{\partial T}{\partial y}\right) - \frac{\partial}{\partial z}\left(k_{33}\frac{\partial T}{\partial z}\right) = Q \tag{4.13}$$

where V is the electric potential, σ_{ij} is the conductivity tensor, T is temperature, k is thermal conductivity, Q is heat source. These equations follow directly from Maxwell's equation and the diffusion equation. In this case,

$$\mathbf{u} = \begin{pmatrix} V \\ T \end{pmatrix} \tag{4.14}$$

$$C = \left(\begin{array}{ccc|ccc} \sigma_{11} & 0 & 0 & 0 & 0 & 0 \\ 0 & \sigma_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & \sigma_{33} & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & k & 0 & 0 \\ 0 & 0 & 0 & 0 & k & 0 \\ 0 & 0 & 0 & 0 & 0 & k \end{array}\right) \tag{4.15}$$

We have

$$\nabla\mathbf{u} = \begin{pmatrix} \nabla V \\ \nabla T \end{pmatrix} = \left(\begin{array}{c} V_{,1} \\ V_{,2} \\ V_{,3} \\ \hline T_{,1} \\ T_{,2} \\ T_{,3} \end{array}\right) \tag{4.16}$$

so that $\nabla \cdot (-C\nabla\mathbf{u})$ is

$$\begin{pmatrix} -(\sigma_{11}V_{,1})_{,1} - (\sigma_{22}V_{,2})_{,2} - (\sigma_{33}V_{,3})_{,3} \\ -(kT_{,1})_{,1} - (kT_{,2})_{,2} - (kT_{,3})_{,3} \end{pmatrix} \tag{4.17}$$

(using $V_{,1} = \partial V/\partial x_1$ etc). And we set $\mathbf{f} = (0, Q)$ and $\mathbf{a} = 0$ to complete the equation set. The Neumann BCs are of the form

$$n_1\sigma_{11}V_{,1} + n_2\sigma_{22}V_{,2} + n_3\sigma_{33}V_{,3} = 0 \tag{4.18}$$

$$n_1kT_{,1} + n_2kT_{,2} + n_3kT_{,3} = 0 \tag{4.19}$$

which are open or natural boundaries. The latter states that no energy flows out of the system (insulator).

It may be noted that there is no coupling between V and T in this problem. In fact we could have just solved for V and T separately. Coupling could be introduced by putting some non-zero off diagonals in (4.15) or by introducing *non-linearity*. For example, the conductivities σ_{11} etc might depend on temperature while the heat source Q might depend on electric field (eg $Q \sim E^2$). ZINC can solve non-linear problems such as this. In linear problems we must set all the components of **C**, **a**, **f**, **q**, **g** to literal constants in the input files (or expressions that evaluate to constants, see Section 5.3). In non-linear problems we can set some or all of the components to expressions involving the dependent variables. See Section 5.5.

4.5 Matrix and component form PDE specification

It is often convenient to consider **C** as a matrix when specifying the problem. Internally, however, ZINC regards it as being a 4 dimensional array of size $N \times d \times N \times d$ where N is the number of

variables and $d = 3$, the number of dimensions. In the above example $N = 2, d = 3$, the matrix (4.15) can be written as

$$\left[\begin{array}{ccc|ccc} C_{1111} & C_{1112} & C_{1113} & C_{1121} & C_{1122} & C_{1123} \\ C_{1211} & C_{1212} & C_{1213} & C_{1221} & C_{1222} & C_{1223} \\ C_{1311} & C_{1312} & C_{1313} & C_{1321} & C_{1322} & C_{1323} \\ \hline C_{2111} & C_{2112} & C_{2113} & C_{2121} & C_{2122} & C_{2123} \\ C_{2211} & C_{2212} & C_{2213} & C_{2221} & C_{2222} & C_{2223} \\ C_{2311} & C_{2312} & C_{2313} & C_{2321} & C_{2322} & C_{2323} \end{array}\right] \tag{4.20}$$

and it is these components C_{ijkl} which must be entered in ZINC's input file. In this way, C may be written as a series of 3×3 "blocks" with the 1st and 3rd component indicating the index of each block. Written in component form, (4.1), (4.2) become,

$$-\left(C_{ijkl}u_{k,l}\right)_{,j} + a_{ik}u_k = f_i, \quad i = 1, \ldots, N \tag{4.21}$$

$$n_j C_{ijkl}u_{k,l} + q_{ik}u_k = g_i, \quad \text{Neumann} \quad i = 1, \ldots, N \tag{4.22}$$

with implied summation over repeat indices. Also, $\mathbf{a}, \mathbf{q}$ are matrices and $\mathbf{f}, \mathbf{g}$ are vectors and their components $a_{ik},\ q_{ik}$ and $f_i,\ g_i$ are entered straightforwardly.

4.6 Multiferroic equations: a more complex example

In multiferroics, frequency domain ($\partial/\partial t \to j\omega$) we may write

$$\sigma_{ij,j} + p_i = -\rho\omega^2 u_i \tag{4.23}$$

$$\nabla \cdot \mathbf{D} = 0 \tag{4.24}$$

$$\nabla \cdot \mathbf{B} = 0 \tag{4.25}$$

$$\nabla \times \mathbf{E} = 0 \tag{4.26}$$

$$\nabla \times \mathbf{H} = 0 \tag{4.27}$$

(with Einstein summation convention). The equations assume no space charge and no current. In this case we can introduce

$$\mathbf{E} = -\nabla V \tag{4.28}$$

$$\mathbf{H} = -\nabla V_m \tag{4.29}$$

$$\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \tag{4.30}$$

so that the curl equations (4.26), (4.27) are automatically satisfied. We use linear constitutive laws as

$$\sigma_{ij} = c^{EH}_{ijkl}\epsilon_{kl} - e_{kij}E_k - e^m_{kij}H_k \tag{4.31}$$

$$D_i = e_{ijk}\epsilon_{jk} + \kappa^{\epsilon H}_{ij}E_j + \alpha_{ij}H_j \tag{4.32}$$

$$B_i = e^m_{ijk}\epsilon_{jk} + \alpha_{ji}E_j + \mu^{\epsilon E}_{ij}H_j \tag{4.33}$$

so that the magnetic and electric equations look just the same. The equations can be written in matrix form as

$$\begin{pmatrix} \boldsymbol{\sigma} \\ \mathbf{D} \\ \mathbf{B} \end{pmatrix} = \begin{pmatrix} c^{EH} & -e^T & -(e^m)^T \\ e & \kappa^{\epsilon H} & \alpha \\ e^m & \alpha^T & \mu^{\epsilon E} \end{pmatrix} \begin{pmatrix} \boldsymbol{\epsilon} \\ \mathbf{E} \\ \mathbf{H} \end{pmatrix} \tag{4.34}$$

Substituting (4.31)-(4.33) in (4.23)-(4.25) and using (4.28)-(4.30), we obtain 5 PDEs

$$\begin{aligned} \left[\frac{1}{2}c^{EH}_{ijkl}(u_{k,l}+u_{l,k}) + e_{kij}V_{,k} + e^m_{kij}V_{m,k}\right]_{,j} + p_i &= -\rho\omega^2 u_i \quad i=1,2,3 \\ \left[\frac{1}{2}e_{ijk}(u_{j,k}+u_{k,j}) - \kappa^{\epsilon,H}_{ij}V_{,j} - \alpha_{ij}V_{m,j}\right]_{,i} &= 0 \\ \left[\frac{1}{2}e^m_{ijk}(u_{j,k}+u_{k,j}) - \alpha_{ji}V_{,j} - \mu^{\epsilon,E}_{ij}V_{m,j}\right]_{,i} &= 0 \end{aligned} \tag{4.35}$$

To input these in ZINC we use the following C matrix (omitting some superscripts for clarity)

$$\left[\begin{array}{ccccccccc|ccc|ccc} c_{11} & c_{16} & c_{15} & c_{16} & c_{12} & c_{14} & c_{15} & c_{14} & c_{13} & e_{11} & e_{21} & e_{31} & e^m_{11} & e^m_{21} & e^m_{31} \\ c_{61} & c_{66} & c_{65} & c_{66} & c_{62} & c_{64} & c_{65} & c_{64} & c_{63} & e_{16} & e_{26} & e_{36} & e^m_{16} & e^m_{26} & e^m_{36} \\ c_{51} & c_{56} & c_{55} & c_{56} & c_{52} & c_{54} & c_{55} & c_{54} & c_{53} & e_{15} & e_{25} & e_{35} & e^m_{15} & e^m_{25} & e^m_{35} \\ c_{61} & c_{66} & c_{65} & c_{66} & c_{62} & c_{64} & c_{65} & c_{64} & c_{63} & e_{16} & e_{26} & e_{36} & e^m_{16} & e^m_{26} & e^m_{36} \\ c_{21} & c_{26} & c_{25} & c_{26} & c_{22} & c_{24} & c_{25} & c_{24} & c_{23} & e_{12} & e_{22} & e_{32} & e^m_{12} & e^m_{22} & e^m_{32} \\ c_{41} & c_{46} & c_{45} & c_{46} & c_{42} & c_{44} & c_{45} & c_{44} & c_{43} & e_{14} & e_{24} & e_{34} & e^m_{14} & e^m_{24} & e^m_{34} \\ c_{51} & c_{56} & c_{55} & c_{56} & c_{52} & c_{54} & c_{55} & c_{54} & c_{53} & e_{15} & e_{25} & e_{35} & e^m_{15} & e^m_{25} & e^m_{35} \\ c_{41} & c_{46} & c_{45} & c_{46} & c_{42} & c_{44} & c_{45} & c_{44} & c_{43} & e_{14} & e_{24} & e_{34} & e^m_{14} & e^m_{24} & e^m_{34} \\ c_{31} & c_{36} & c_{35} & c_{36} & c_{32} & c_{34} & c_{35} & c_{34} & c_{33} & e_{13} & e_{23} & e_{33} & e^m_{13} & e^m_{23} & e^m_{33} \\ \hline e_{11} & e_{16} & e_{15} & e_{16} & e_{12} & e_{14} & e_{15} & e_{14} & e_{13} & -\kappa_{11} & -\kappa_{12} & -\kappa_{13} & -\alpha_{11} & -\alpha_{12} & -\alpha_{13} \\ e_{21} & e_{26} & e_{25} & e_{26} & e_{22} & e_{24} & e_{25} & e_{24} & e_{23} & -\kappa_{21} & -\kappa_{22} & -\kappa_{23} & -\alpha_{21} & -\alpha_{22} & -\alpha_{23} \\ e_{31} & e_{36} & e_{35} & e_{36} & e_{32} & e_{34} & e_{35} & e_{34} & e_{33} & -\kappa_{31} & -\kappa_{32} & -\kappa_{33} & -\alpha_{31} & -\alpha_{32} & -\alpha_{33} \\ \hline e^m_{11} & e^m_{16} & e^m_{15} & e^m_{16} & e^m_{12} & e^m_{14} & e^m_{15} & e^m_{14} & e^m_{13} & -\alpha_{11} & -\alpha_{21} & -\alpha_{31} & -\mu_{11} & -\mu_{12} & -\mu_{13} \\ e^m_{21} & e^m_{26} & e^m_{25} & e^m_{26} & e^m_{22} & e^m_{24} & e^m_{25} & e^m_{24} & e^m_{23} & -\alpha_{12} & -\alpha_{22} & -\alpha_{32} & -\mu_{21} & -\mu_{22} & -\mu_{23} \\ e^m_{31} & e^m_{36} & e^m_{35} & e^m_{36} & e^m_{32} & e^m_{34} & e^m_{35} & e^m_{34} & e^m_{33} & -\alpha_{13} & -\alpha_{23} & -\alpha_{33} & -\mu_{31} & -\mu_{32} & -\mu_{33} \end{array}\right] \tag{4.36}$$

where we use the matrix representation

tensor	11	22	33	23,32	13,31	12,21
matrix	1	2	3	4	5	6

so that $c_{1213} = c_{65}$ etc. Of course c is not to be confused with C, the ZINC PDE matrix. The C matrix above is such that

$$\nabla\cdot(C\nabla\mathbf{u}) = \begin{pmatrix} \left[\frac{1}{2}c_{1jkl}(u_{k,l}+u_{l,k}) + e_{k1j}V_{,k} + e^m_{k1j}V_{m,k}\right]_{,j} \\ \left[\frac{1}{2}c_{2jkl}(u_{k,l}+u_{l,k}) + e_{k2j}V_{,k} + e^m_{k2j}V_{m,k}\right]_{,j} \\ \left[\frac{1}{2}c_{3jkl}(u_{k,l}+u_{l,k}) + e_{k3j}V_{,k} + e^m_{k3j}V_{m,k}\right]_{,j} \\ \left[\frac{1}{2}e_{ijk}(u_{j,k}+u_{k,j}) - \kappa_{ij}V_{,j} - \alpha_{ij}V_{m,j}\right]_{,i} \\ \left[\frac{1}{2}e^m_{ijk}(u_{j,k}+u_{k,j}) - \alpha_{ji}V_{,j} - \mu_{ij}V_{m,j}\right]_{,i} \end{pmatrix} \tag{4.37}$$

Rearranging (4.1) gives,

$$\nabla \cdot (C\nabla \mathbf{u}) + \mathbf{f} = a\mathbf{u} \tag{4.38}$$

so that

$$a = \begin{pmatrix} -\rho\omega^2 & 0 & 0 & 0 & 0 \\ 0 & -\rho\omega^2 & 0 & 0 & 0 \\ 0 & 0 & -\rho\omega^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{4.39}$$

and $f_i = p_i$ gives the correct set of equations (4.35). It is easy to check that the Neumann boundary condition (4.2) (with $q = g = 0$) corresponds physically to

$$n_j\sigma_{ij} = 0, \quad n_iD_i = 0, \quad n_iB_i = 0 \tag{4.40}$$

i.e., zero charge, zero magnetic flux and zero traction at the boundaries. These are good choices for an open boundary. This example if quite complicated and the input file, `filename.zin` will be very long. It is likely that the user will write a preprocessor program to generate this file.

Chapter 5

Zinc (core solver)

ZINC has two basic input files, a geometry file (`filename.mtf`) specifying the system mesh; and a materials file (`filename.zin`) specifying material properties, physics, initial state, boundary conditions and convergence information. There are three optional files: a file containing constants (`filename.con`); a restart file `filename.rst` for specifying the initial state if not supplied in `filename.zin`, see `key_rdu`; and `filename.dll` which contains non-linear functions if needed. Regarding the restart file, to continue from a previous run, copy `filename.zou` to `filename.rst`. In this case, you will need to set `key_rdu=1` in file `filename.zin`.

ZINC outputs two major files (`filename.zou, filename.zls`). The output file `filename.zou` contains the value of each of the variables solved for at each node (in static/steady state problems, this file contains just the final snapshot, in transient problems it contains several intermediate snapshots showing the time evolution, see `nstride` below). `filename.zls` contains the full set of input data and information on the convergence etc of the run.

The information in `filename.zou` is not directly useable for graph plotting. Accordingly a post processor has been prepared, ZPP, which reads `filename.zou` as prepared by ZINC and outputs a series of scans through the data, see Chapter 6.

ZINC also, optionally, exports files in ParaView format (see `key_export` below). Paraview is a powerful and free post processor that allows 3-D visualization of the simulation results. For static runs, just one paraview file, `filename.vtk`, is output corresponding to the final state. In transient runs, snapshots are output every `nstride` timesteps. These are written to files `filenamexx.vtk`, where xx is 1,2,3...

The normal procedure for using ZINC is

1. Prepare `filename.mtf` (generated by ZMESH or another program), `filename.zin, filename.con` for simulation

2. Run ZINC.

3. Prepare `filename.zpp` for post processing scans

4. Run ZPP to generate scans through the data. ZPP can automatically create graphs or these files can be plotted with a graph plotter or spreadsheet of the user's preference.

5. Alternatively, results can be output and viewed with Paraview

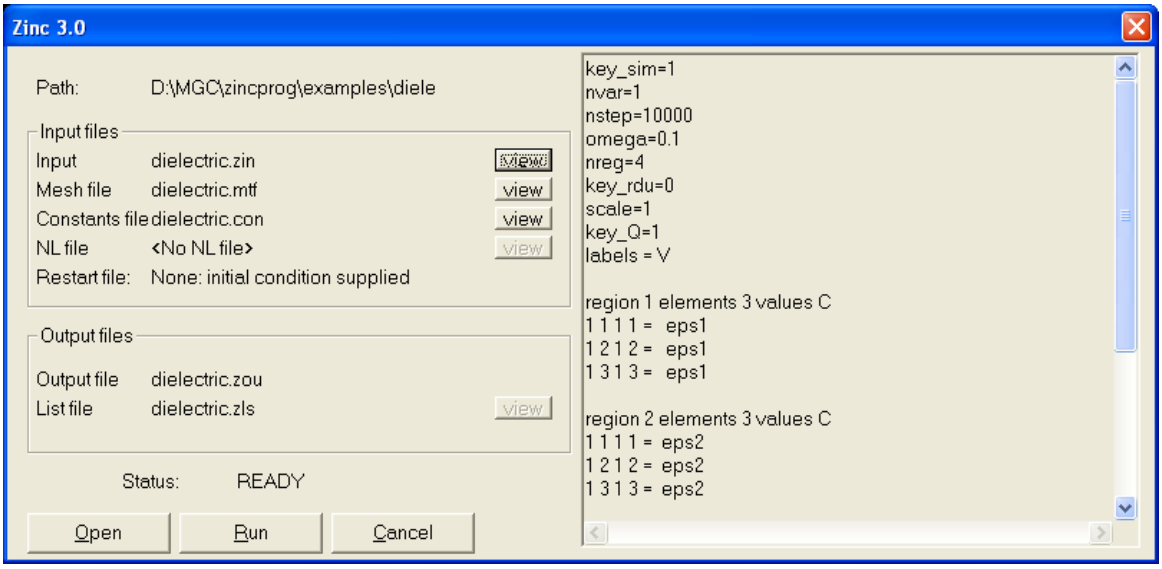


Figure 5.1: Program ZINC

If a different set of line/plane scans is needed, just update `filename.zpp` and run ZPP again. It is not necessary to run ZINC again if you simply want to see the data along a different direction!

The ZINC program is shown in Figure 5.1. The program allows the user to marshal and view the various input and output files. Click "open" to select an input (ZIN) file. You can view files using the "view" buttons. Then run the simulation using "run".

ZINC can also be run at the command line using

```
zinc filename
```

5.1 Mesh definition file file.mtf

ZINC works with a 3-D *structured mesh* of hexahedrons (squashed cuboids). The strucured mesh has the same topology as a regular cubic grid so that no connection table is needed. It is always guaranteed that node (I, J, K) will be connected to $(I+1, J, K)$ etc. Every node in the interior is surrounded by 8 elements. The input file `zinc.mtf` is therefore very simple, it begins like this

```
IMax:       20
JMax:       20
KMax:       27

    I       J       K         x           y           z      RegNo RegUp
=============================================================================
       0       0       0 -3.0000E+02 -3.0000E+02 -2.5000E+01     3     1
       1       0       0 -2.4531E+02 -3.0000E+02 -2.5000E+01     3     1
```

```
      2       0       0 -1.9140E+02 -3.0000E+02 -2.5000E+01     3     1
      3       0       0 -1.4003E+02 -3.0000E+02 -2.5000E+01     3     1
      4       0       0 -9.4604E+01 -3.0000E+02 -2.5000E+01     3     1
      5       0       0 -5.9265E+01 -3.0000E+02 -2.5000E+01     3     1
      6       0       0 -3.5648E+01 -3.0000E+02 -2.5000E+01     3     1
:
:
```

Nodes are numbered `(I,J,K)=(0,0,0)` to `(IMax,JMax,KMax)`. Each row in the table gives the (I, J, K) index of the node, its coordinate, its *region number* and the region number of the element in the positive x, y, z directions (`RegUp`). A detailed description of the `.mtf` file format is given in Appendix B. In practice `file.mtf` is normally generated by ZMESH.

Once nodes and region numbers have been set in the `.mtf` file, the materials file, `filename.zin`, sets the material properties associated with these regions. The *elements* are given values **C, a, f** according to region numbers while *nodes* can be fixed at specified values according to their region numbers giving Dirichlet boundaries. Nodes can be fixed within the volume not just over the boundary, it is possible to set only certain variables while leaving others free on a given node. Finally Neumann boundaries are set using **q, g** values.

5.2 Material/physics file `filename.zin`

The file consists of several parts, which may be given in any order:

1. Control variables of the form `variable=value`. This includes number of time steps to run, the simulation type etc.

2. Region specification blocks. Associates material properties and physics with each region number. These blocks start with `region xx elements...` or `region xx nodes...`, see below.

3. Surface statements applying Neuman boundary conditions

4. The initial condition. This is followed by `nvar` lines of specifying the initial state of each simulation variable.

The above information may be given in any order. Line spacing is unimportant and comment lines may be inserted beginning with `!`. Lines may be continued using the ampersand (&) character, for example:

```
  key_sim= &
1
```

is the same as

```
  key_sim=1
```

5.2.1 Control variables

Some control variable are compulsory and ZINC will report an error if they are not set. Others are optional and will take on default values if not set.

Compulsory control variables: These are `nvar,nreg,key_sim,nstep`. Also, if `key_sim=2` (transient simulation), the time step `tstep` must be set.

nvar Number of variables. Eg, 5 in multiferroics.

nstep number of iteration steps. With `key_sim=1,2` this is the total number of steps with non-linear elements being updated periodically, according to `nstrideNL`. In `key_sim=3,4,5,6`, it is the number of times the elements are updated[1]

nreg Number of regions in file. `Zinc.mtf` should contain the same number of regions

tstep Time step for transient problems.

key_sim 1: Static or steady state run; 2 transient run; 3 static run with GMRES solver (diagonally scaled); 4 GMRES solver (Incomplete LU factorisation); 5 Biconjugate Gradient solver (Diagonally scaled); 6 Biconjugate Gradient solver (Incomplete LU factorisation)

Optional variables: These are `omega, key_rdu, scale, nstride, nstrideNL, labels`. Some other control variables, which are only of interest for debugging and code development, are listed in Appendix C.

omega Successive over-relaxation parameter. Less than 1, of order 0.1. (default 0.1)

key_rdu 0: Start from initial condition in the `init` section of `filename.zin`. 1: read `filename.rst` to define initial state. If you want to continue from a pervious run, copy `filename.zou` to `filename.rst` (If the previous simulation was transient, `filename.zou` will consist of several snapshots. In this case ZINC automatically reads the last one of these from `filename.rst` and continues from that). (Default 0)

scale factor to multiply distances found in `zinc.mtf` to put them in metres (or whatever distance unit in implied in the PDEs that have been set). E.g. if the dimensions in the `zinc.mtf` file are mm set scale to 0.001. (Default 1).

nstride Steps between output of convergence information and writing snapshots (in transient problems) (default 10)

nstrideNL Steps between updating finite element matrices during non-linear runs. In non-linear problems, the matrices must be updated to account for changing material properties. Only used if `key_sim=1,2` (default 10)

key_export . 0: No export. 1: Export to Paraview format `.vtk` files. (default 0)

[1] This is unfortunately a bit confusing. In the case of `key_sim=1,2`, the system runs for `nstep` timesteps and, in the case of non-linear systems, updates the matrices every `nstride_NL` steps. Other solvers simply converge based on `tol` and `itmax`. For linear problems, `nstep` is not used; for non-linear, `nstep` is the number of non-linear iterations

labels List of `nvar` labels for the variables being simulated. Eg, in a thermo-electric simulation, we might have `labels T V`

tol, itmax Used only when `key_sim=3,4,5,6`. `tol` is the convergence tolerance and `itmax` is the maximum number of iterations carried out by these linear solvers.

5.2.2 Region specification blocks

These have the form

```
region i [keyword] N values [matrix name]
```

If keyword is "elements" specify material properties of elements with region number `i`. The matrix name, `C, a` or `f` is given and number of values `N` to be specified. There then follows a list of `N` entries of form:

```
<list of indices> = value
```

C has 4 components so an entry in the list might be

```
    1    1    1    1 = 0.31100E+11
```

which specifies $C_{1111} = 0.31100 \times 10^{11}$ (SI units). Note that expressions may be entered in place of literal constants, a facility which allows spacial variation of material properties and/or non-linearity. See Section 5.3.

An alternative, if `labels` has been specified, is to enter the variable names and the directions `x,y,z`. Thus we might have

```
  V x V x = 0.31100E+11
```

This still sets $C_{1111} = 0.31100 \times 10^{11}$ as before, but may be more helpful as it gives a clearer idea what the meaning of this C element is.

Coefficient a has 2 components so and entry in the list might be

```
  1 1 = -3.03983816e15 OR
  V V = -3.03983816e15
```

which specifies $a_{11} = -3.03983816 \times 10^{15}$ (SI units). Coefficient f has 1 component so an entry might be

```
  1 = 0.5 OR
  V = 0.5
```

which specifies $f_1 = 0.5$ (SI units)

A complete region entry would look like

```
region 2 elements 3 values a
1 1 = -3.03983816e15
2 2 = -3.03983816e15
3 3 = -3.03983816e15
```

Note: Zero values need not be entered, these are assumed by default. The full specification of **C**, **a**, **f** will be written in `filename.zls`, it is advisable to check this.

If the keyword is "nodes" then specify nodes to have fixed values of one or more variables. N is the number of fixed values, `[matrix name]` is not used. There then follows a list of fixed variables of form variable number (or symbol) then value. Eg, to fix variables 4 and 5 in region 9 use:

```
region 9 nodes 2 values
4 = 0.04
5 = 0
```

or, if `labels` has been set

```
region 9 nodes 2 values
T = 0.04
V = 0
```

(for example). The latter form is easier to read.

This fixes, $u_4 = T = 0.04$ and $u_5 V == 0$ in region 9 nodes. Variables not specified default to *not* being fixed. The specification of all nodes and whether they are fixed is written out `filename.zls`.

5.2.3 Specifying Neumann boundaries at surfaces

So far we have set material properties/physics within regions and Dirichlet boundaries on nodes. The other boundary condition is Neumann boundary which has the general form

$$n_j C_{ijkl} u_{k,l} + q_{ik} u_k = g_i \tag{5.1}$$

The q and g values default to zero. To set them non-zero, we identify a surface between to volumetric regions (see Figure 3.6) and attach parameters using the command

```
surface i j N values [matrix name]
```

where i and j are the two regions, N is the number of entries to follow and "matrix name" must be "g" or "g". A typical example is

```
surface 1-2 3 values g
   1 = 1.0
   2 = 2.0
   3 = 3.0
```

If labels have been defined, these can be used as well. Eg in an electrostatic problem with labels (displacements) `u, v, w`

```
surface 1-2 3 values g
   u = 1.0
   v = 2.0
   w = 3.0
```

As shown in Figure 3.6, the simulation is conceptually surrounded by regions called XMAX etc. Thus, 1-XMAX is the surface between region 1 and the maximum-x edge of the simulation.

Name	Meaning
pi	The constant π
i	The constant $\sqrt{-1}$
x	x position in space
y	y position in space
z	z position in space
nx	x-component of unit normal (used for **q**, **g** only)
ny	y-component of unit normal (used for **q**, **g** only)
nz	z-component of unit normal (used for **q**, **g** only)
u1	first variable value
u2	second variable value
:	:
u1x	derivative of first variable with respect to x
u1y	derivative of first variable with respect to y
u1z	derivative of first variable with respect to z
u2x	derivative of second variable with respect to x
u2y	derivative of second variable with respect to y
u2z	derivative of second variable with respect to z
:	:

Table 5.1: Built in variables which can be used in ZINC expressions. If the user defines the names of variables, these will be used in place of `u1, u2` etc. The user may also reference constants in the `.con` file.

5.2.4 Initial state specification

It is also necessary to specify the initial state of the system. For example, in a thermo-electric problem, with `labels T, V` we could have

```
init
   T=1
   V=0
```

which sets the initial temperature to 1 and the initial voltage to zero. It is also possible to set the initial state from a previous ZINCrun, by setting `key_rdu=1`. In this case, a `file.rst` must be present. Of course, the user could write a program to generate his own initial state.

5.3 Expressions

Instead of entering a literal constant like `1.0`, it is possible, in **C**, **a**, **f**, **q**, **g**, nodal and initial specifications, to enter mathematical expressions. The expression may depend on: the constants in `filename.con`; the built-in variables `pi=3.14159, i=sqrt(-1)`; spatial variables `x,y,z`; and variables corresponding to the dependent variables to be solved for. These last are called `u1,u2,...u(nvar)`. Their derivatives are also available and are called `u1x,u1y,u1z, u2x,u2y,u2z...`. However, if `labels` has been set, these names are used instead. Thus, in a thermo-electric system, with variables `T,V`, the standard variables are `T, V, Tx, Ty, Tz, Vx, Vy, Vz`. The full set of built-in variables in shown in Table 5.1.

Built-in variables `x,y,z` are the spatial coordinate in the coordinate system specified in `filename.mtf`. If expressions are given in terms of dependent variables $u1$ etc or their derivatives, the simulation automatically becomes *non-linear*. The functions `sin, cos, tan, sqrt, exp, log, ln, abs, ang, real, imag, conjg, complex` may be used. Note that `log` is $\log_{10}$ while `ln` is $\log_e$. Complex numbers may be constructed as `a+b*i` or with the function `complex`: `complex(a,b)`. Note that, although complex expressions are allowed, all expressions must evaluate to real since ZINC operates with real numbers only. If an expression is complex, it will be truncated to real by discarding the imaginary part.

Examples of legal expressions include:

```
1                                  ! same as 1.0, 1e0
1+h/2                              ! h must be present in filename.con
1e-6*(1+exp(-(x-x0)^2/(2*sig^2))) ! Gaussian, x0, sig must be in filename.con
u1^2+u2y/u3z                       ! Depends on solution variables: non-linear
```

Allowed operators include addition (+), multiplication (*), subtraction (-), division (/), exponentiation ($\hat{}$).

There are some restrictions on the size of expressions

1. The total string length of each expression is limited to 1000 characters (including blank spaces)
2. The total number of "items" in each expression is limited to 350. Here, an item is: a variable, a constant, an operator, an open or close bracket, a function like sin, cos, exp...
3. The maximum number of variables is 1000.

In practice these restrictions still allow highly complex equations. If your expressions are getting more complex than this, you should consider using a DLL to specify the expression. See Section 5.5.

There are some restrictions on the type of expressions for each specification:

1. **q**, **g** specifications and node specifications (Dirichlet boundaries) may only be in terms of variables *not* their derivatives. This is because derivative quantities are not well defined on element boundaries or nodes.
2. Initialisation expressions may only be in terms of x,y,z and constants

5.4 The constants file, `file.con`

It is often convenient to define constants in the `file.con` file. These can easily be changed between simulation without getting into the details of the `file.zin` file (which also contains the physics of the system). For instance, in an electrostatic simulation, we might have the following `.con` file.

```
eps0=8.854e-12
eps1=eps0
eps2=2*eps0
```

thus setting up permittivities in various regions. In the `file.zin` file, we could then have

```
region 1 elements 3 values C
   1 1 1 1 = eps1
   1 2 1 2 = eps1
   1 3 1 3 = eps1

region 2 elements 3 values C
   1 1 1 1 = eps2
   1 2 1 2 = eps2
   1 3 1 3 = eps2
```

The `.con` file contains a series of lines of the form

```
var = value
```

Constants may be defined `in terms of pervious constants` but not later ones. Thus the following `.con` file would be illegal

```
eps1=eps0     ! eps0 not yet defined
eps2=2*eps0
eps0=8.854e-12
```

The usual expression rules apply for expressions in the constants file.

5.5 Advanced, non-linear simulations

For linear simulations, each of the numbers specifying **C**, **a**, **f** **q**, **g** is: either a constant or evaluates to a constant OR depends only on `x,y,z`. In non-linear simulations, one or more **C**, **a**, **f** **q**, **g** numbers (or Dirichlet boundary values) depends on the solved-for variables (`u1` etc) through an expression. These expressions allow simple non-linearity but there is a more advanced technique when the **C**, **a**, **f** **q**, **g** expressions become complicated, perhaps requiring an actual computer program to generate. In this case the user should enter a *token* beginning with `$` e.g., `$copper_stiffness` instead of a number. The token is passed through to functions `Cfun, afun, ffun, gfun, qfun, BCfun` which the user must provide in `file.dll`. `BCfun` is used for Dirichlet boundary conditions, i.e., for node specification "`region x nodes ...`". An example of `ffun` in Fortran would be

```
function ffun(label,x,y,z,ur,dur,nvar,istep)

  implicit none
  character(*) label
  integer nvar
  double precision Cfun,x,y,z,ur(nvar),dur(nvar,3)

  if (label.eq.'$ohmic_heating') then
      ffun=dur(1,1)**2+dur(1,2)**2+dur(1,3)**2
```

```
      ! other options...

  endif

end function ffun
```

In C, the function `ffun` would look something like this

```
double ffun(char *label, double *x, double *y, double *z,
            double ur[1], double dur[3][1], int *nvar, int *istep, int length)
{
  double Ex,Ey,Ez;

  if (equal(label,length,"$ohmic_heating"){
      Ex=dur[0][0];
      Ey=dur[1][0];
      Ez=dur[2][0];

      return Ex*Ex+Ey*Ey+Ez*Ez;
  }

  // other options...

}
```

Note that the string passed in is not null-terminated but of fixed length `length` and is hence dealt with using our own `equal` function as shown in Figure 5.2. Also the C `dur` matrix is transposed compared to the Fortran matrix. You need to be aware of issues like this if you are using a different language (read your compiler manual!). Chapter 3 of the Tutorial Manual shows a fuel cell simulation using Fortran and C non-linear functions using the free gcc compiler.

In this example, the program substitutes the value

$$\left(\frac{\partial u_1}{\partial x_1}\right)^2 + \left(\frac{\partial u_1}{\partial x_2}\right)^2 + \left(\frac{\partial u_1}{\partial x_3}\right)^2 \tag{5.2}$$

wherever the token `$ohmic_heating` appears in `filename.zin`. For example in an electrostatic run, $u_1 = V$, the potential so the above expression is $|E|^2$. In functions `cfun, afun, ffun, qfun, gfun`, `ur(i)`$= u_i$, `dur(i,j)`$= \partial u_i/\partial x_j$.

The variables passed to the non-linear functions are as follows

label A string containing the token specified in the input file, including the initial $.

x,y,z The current spatial position (given by reference to the meshing (double precision[2])

ur Array of length `nvar` containing the current solution at (x,y,z), `ur(i)`$= u_i$ (double precision)

dur Array of size `dur(nvar,3)` so that `dur(i,j)`$= \partial u_i/\partial x_j$ at (x,y,z) (double precision)

[2] 8 byte reals

```
int equal(char *s, int length, char *t)
{

  int i,len1,len2;

  for (i=0;i<length;i++){
    if (s[i]==' ') break;
  }

  len1=i;

  for (i=0;i<length;i++){
    if (t[i]=='\0') break;
  }

  len2=i;

  if (len1==len2){
    for (i=0;i<len1;i++)
      if (s[i]!=t[i]) return 0;

    return 1;
  }
  else
    return 0;
}
```

Figure 5.2: A simple function to compare strings `s` (fixed length `length`) and `t` (null terminated)

nvar Number of variables (integer)

istep The current iteration step. In transient problems the current time is `istep*tstep` where `tstep` is described in Section 5.2.1. `istep` may be useful in static problems as well since the non-linear routines can use it to find out when the ZINC matrices have been updated.

nx,ny,nz (only available when forming **q** and **g** matrices. The current outward surface unit normal pointing *from* the first specified region *to* the second. eg for a surface beginning `surface 1-2 3 values g`, the normal provided would be *from* region 1 *to* region 2. (double precision)

The full template the for the non-linear functions in `file.dll` is shown in Figure 5.3. The function `scanfun` is used by ZPP, which is described in Chapter 6. The full template for C non-linear functions is given in Figure 5.4.

Note that derivative quantities are available for forming **C**, **a**, **f** matrices but not for **q**, **g** matrices (since derivatives are not well defined on element boundaries). On the other hand, only `qfun, gfun` have access to the local surface normal since this concept is only meaningful on a surface.

5.6 Examples of zinc input files

Refering to the simple "sphere in a cube" geometry shown in Figure 3.4, Figure 5.5 shows a simple linear system to solve an electrostatic problem with 1 V applied across the system. The inner sphere has rel. permittivity 2 and the outer area rel. permittivity 1. The initial voltage is 0 V.

In the second example, Figure 5.6, the permittivity depends on the electric field as $(1 + E/|E0|) * \epsilon$. In this example, we have chosen a better guess for the initial voltage: a linear variation between 0 (at $z = -h/2$, say) and 1 V (at $z = h/2$) on the top and bottom plates.

In the third example, Figure 5.7, the exact same simulation is carried out using non-linear functions in `dielectric.dll`. In this case, ZINC will detect the presence of `dielectric.dll` and link it to the ZINC core.

5.7 Zinc: output files

filename.zls Describes specification of run including **C**, **a**, **f** **q**, **g** values for each region and which nodes are fixed. Also shows initial and final distribution of energy in different regions. The program actually calculates energy in two different ways which should give the same answer. For checking purposes, this file lists how many times each element was used in forming the FE matrix. Each element should be used 64 times.

filename.zou Value of each variable at each node. This can be read by ZPP in post processing. The format is I, J ,K, variable number and value. To continue another run where you left off, copy this file to `filename.rst` and set `key_rdu=1`

filenamexx.vtk Snapshots in Paraview format. These are output every `nstride` timesteps if `key_export=1`. In static runs, only one `.vtk` file is output at the end of the simulation.

```
function Cfun(label,x,y,z,ur,dur,nvar,istep)
  character(*) label
  integer nvar,istep
  double precision Cfun,x,y,z,ur(nvar),dur(nvar,3)
end function Cfun

function afun(label,x,y,z,ur,dur,nvar,istep)
  character(*) label
  integer nvar,istep
  double precision afun,x,y,z,ur(nvar),dur(nvar,3)
end function afun

function ffun(label,x,y,z,ur,dur,nvar,istep)
  character(*) label
  integer nvar,istep
  double precision ffun,x,y,z,ur(nvar),dur(nvar,3)
end function ffun

function qfun(label,x,y,z,nx,ny,nz,ur,nvar,istep)
  character(*) label
  integer nvar,istep
  double precision qfun,x,y,z,nx,ny,nz,ur(nvar)
end function qfun

function gfun(label,x,y,z,nx,ny,nz,ur,nvar,istep)
  character(*) label
  integer nvar,istep
  double precision gfun,x,y,z,nx,ny,nz,ur(nvar)
end function gfun

function BCfun(label,x,y,z,ur,nvar,istep)
  character(*) label
  integer nvar,istep
  double precision BCfun,x,y,z,ur(nvar)
end function BCfun

function scanfun(label,x,y,z,nx,ny,nz,ur,dur,nvar)
  character(*) label
  integer nvar
  double precision scanfun,x,y,z,nx,ny,nz,ur(nvar),dur(nvar,3)
end function scanfun
```

Figure 5.3: Template for Fortran non-linear functions, `file.dll`

```
double cfun(char *label, double *x, double *y, double *z,
     double ur[1], double dur[3][1], int *nvar, int *istep, int length)
{
}

double afun(char *label, double *x, double *y, double *z,
     double ur[1], double dur[3][1], int *nvar,int *istep, int length)
{
}

double ffun(char *label, double *x, double *y, double *z,
      double ur[1], double dur[3][1], int *nvar, int *istep, int length)
{
}

double qfun(char *label, double  *x, double  *y, double  *z,
                         double *nx, double *ny, double *nz,
      double ur[1], int *nvar, int *istep, int length)
{
}

double gfun(char *label, double  *x, double  *y, double  *z,
                         double *nx, double *ny, double *nz,
      double ur[1], int *nvar, int *istep, int length)
{
}

double BCfun(char *label, double *x, double *y, double *z,
      double ur[1], int *nvar, int *istep, int length)
{
}

double scanfun(char *label, double  *x, double  *y, double  *z,
                            double *nx, double *ny, double *nz,
      double ur[1], int *nvar, int length)
{
}
```

Figure 5.4: Template for C non-linear functions, `file.dll`. Here we have assumed that there is 1 variable. The C functions receive an additional variable, `length`, which is the length of the string `label`. This string is *not* null terminated.

```
dielectric.con:
===============
  eps0=8.854e-12


dielectric.zin
==============
  nvar = 1
  nreg = 3
  labels = V
  <other global commands>
  :

  region 1 elements 3 values C
    V x V x = eps0
    V y V y = eps0
    V z V z = eps0

  region 2 elements 3 values C
    V x V x = 2*eps0
    V y V y = 2*eps0
    V z V z = 2*eps0

  region 3 nodes 1 value
    V = 1

  region 4 nodes 1 value
    V = 0

  init
    V=0
```

Figure 5.5: Simple linear electrostatic simulation, cf Figure 3.4

```
dielectric.con:
===============
  eps0=8.854e-12
  eps1=eps0
  eps2=2*eps0
  E01=1000   ! V/m
  E02=2000   ! V/m
  h=1e-3     ! m

dielectric.zin
==============
  nvar = 1
  nreg = 3
  labels = V
  <other global commands>
  :

  region 1 elements 3 values C
    V x V x = (1+sqrt(Vx^2+Vy^2+Vz^2)/E0)*eps1
    V y V y = (1+sqrt(Vx^2+Vy^2+Vz^2)/E0)*eps1
    V z V z = (1+sqrt(Vx^2+Vy^2+Vz^2)/E0)*eps1

  region 2 elements 3 values C
    V x V x = (1+sqrt(Vx^2+Vy^2+Vz^2)/E0)*eps2
    V y V y = (1+sqrt(Vx^2+Vy^2+Vz^2)/E0)*eps2
    V z V z = (1+sqrt(Vx^2+Vy^2+Vz^2)/E0)*eps2

  region 3 nodes 1 value
    V = 1

  region 4 nodes 1 value
    V = 0

  init
    V=0.5*(z/h+1)
```

Figure 5.6: Non-linear dielectric simulation

```
dielectric.con:
===============
  h=1e-3    ! m

dielectric.zin
==============
  nvar = 1
  nreg = 3
  labels = V
  <other global commands>
  :

  region 1 elements 3 values C
    V x V x = $epsilon1
    V y V y = $epsilon1
    V z V z = $epsilon1

  region 2 elements 3 values C
    V x V x = $epsilon2
    V y V y = $epsilon2
    V z V z = $epsilon2

  region 3 nodes 1 value
    V = 1

  region 4 nodes 1 value
    V = 0

  init
    V=0.5*(z/h+1)

dielectric.dll
==============

  function Cfun(label,x,y,z,ur,dur,nvar,istep)
    character(*) label
    double precision Cfun,x,y,z,ur(nvar),dur(nvar,3)
    integer nvar,istep

    double precision, parameter :: eps0=8.854e-12
    double precision, parameter :: eps1=eps0,eps2=eps0*2
    double precision, parameter ::E10=1000, E20=2000
    double precision E

    E=sqrt(dur(1,1)**2+dur(1,2)**2+dur(1,3)**2)

    if (label.eq.'$epsilon1') then
       Cfun=(1+E/E10)*eps1
    else if (label.eq.'$epsilon2') then
       Cfun=(1+E/E20)*eps2
    endif
  end function Cfun
```

Figure 5.7: Non-linear dielectric simulation

Chapter 6

Zpp: the Zinc post processor

The ZINC Post Processor, ZPP, is shown in Figure 6.1. Use "Open" to select a `file.zpp` input file (see below), then "Run" to perform the post processing. The lower list box shows the output files generated. Clicking on one and selecting "graph" shows a graph of the line or plane scan selected (this button is deactivated for integrals since these do not generate a graph). Again, individual files can be examined using the "view" buttons.

ZPP allows complex views to be taken through the data and can also perform integrations. You can plot the raw solved-for variables, their derivatives or any function of these according to the usual rules for expressions, Section 5.3. However, there is a new conditional expression type, described in Section 6.2. If you want to plot an additional view, just add it to the input file and re-run ZPP. There is no need to re-run ZINC itself just to get a different line scan! A basic view of the simulation output can also be obtained using ZMESH, Section 3.1.

6.1 Zpp input files

ZPP reads `filename.zin, filename.mtf, filename.con` just as ZINC does. It also reads its own file `filename.zpp` which has the form

```
<global commands>
calculation 1
calculation 2
etc
```

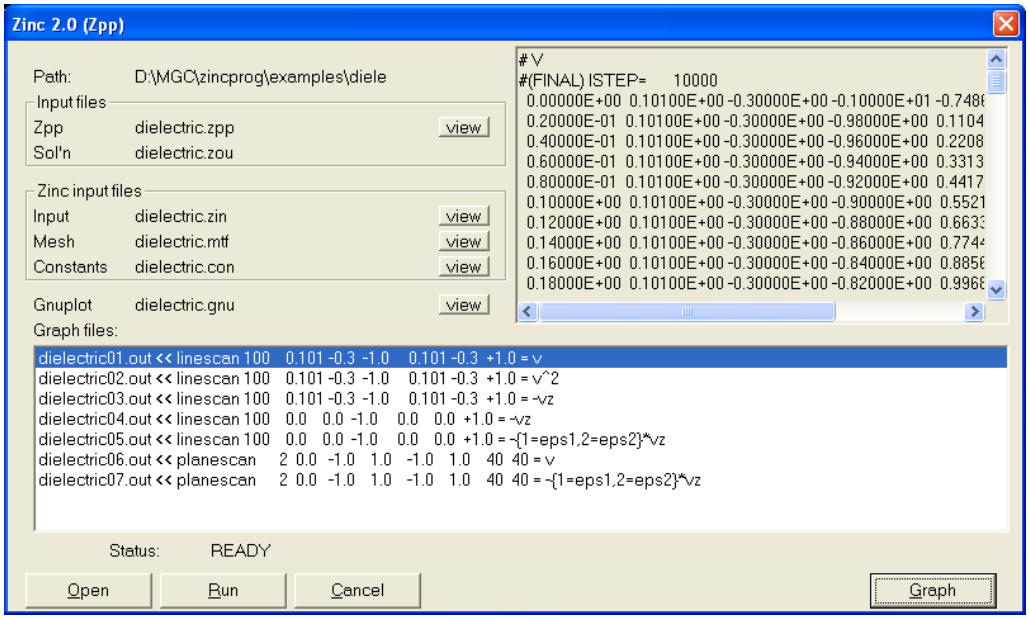
The global commands are

ftol tolerance for finding points in elements. Must be less then 1, typically order 1e-3. This is used when the program tries to evaluate variable values at a point (x, y, z) e.g. in line/plane scans. If the point lies on the interface between elements there is ambiguity and this tolerance is needed to find a value. (default 0.001)

key_plot 0: do not plot; 1: automatically create Encapsulated Postscript files (`.eps`) using gnuplot (which must be installed); 2: automatically create Enhanced Metafiles (`.emf`)

Calculations have the form

```
{calculation} [parameters] = expression
```


Zinc 2.0 (Zpp)
Path: D:\MGC\zincprog\examples\diele
Input files
Zpp dielectric.zpp view
Sol'n dielectric.zou
Zinc input files
Input dielectric.zin view
Mesh dielectric.mtf view
Constants dielectric.con view
Gnuplot dielectric.gnu view
Graph files:
dielectric01.out << linescan 100 0.101 -0.3 -1.0 0.101 -0.3 +1.0 = v
dielectric02.out << linescan 100 0.101 -0.3 -1.0 0.101 -0.3 +1.0 = v^2
dielectric03.out << linescan 100 0.101 -0.3 -1.0 0.101 -0.3 +1.0 = -vz
dielectric04.out << linescan 100 0.0 0.0 -1.0 0.0 0.0 +1.0 = -vz
dielectric05.out << linescan 100 0.0 0.0 -1.0 0.0 0.0 +1.0 = -{1=eps1,2=eps2}*vz
dielectric06.out << planescan 2 0.0 -1.0 1.0 -1.0 1.0 40 40 = v
dielectric07.out << planescan 2 0.0 -1.0 1.0 -1.0 1.0 40 40 = -{1=eps1,2=eps2}*vz
Status: READY
Open
Run
Cancel
Graph

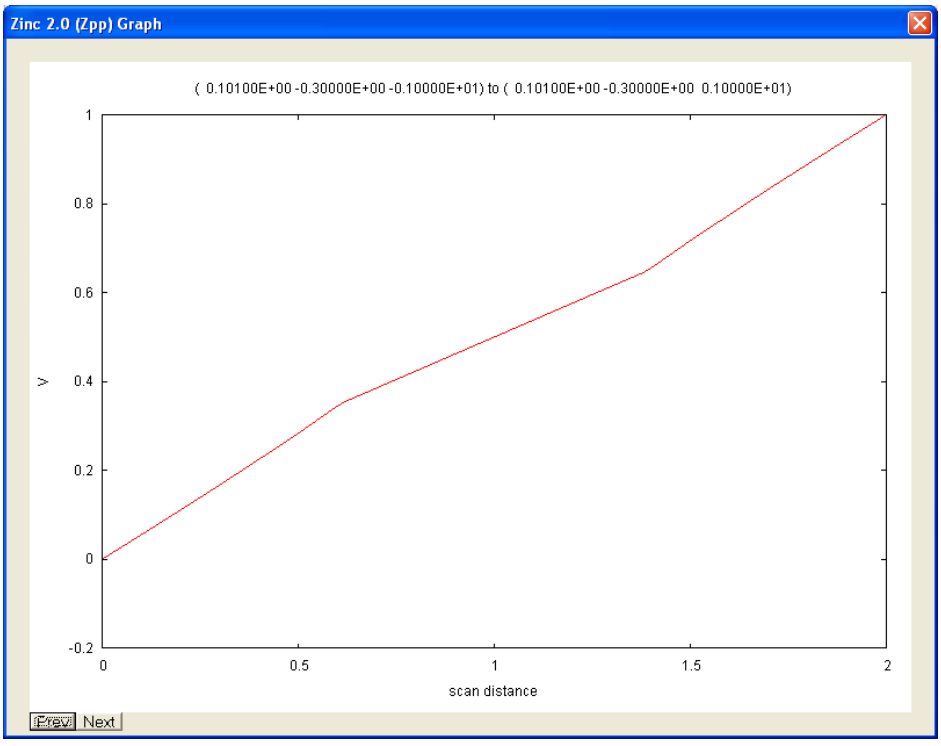


Figure 6.1: Program Zpp, top, and automatically generated graph, bottom.

The following calculations are supported

linescan Perform a linescan through the data. The parameters are `nline x1 y1 z1 x2 y2 z2` where `nline` is the number of points between coordinates (x1,y1,z1) and (x2,y2,z2)

planescan Perform a planescan through the data. The parameters are `inorm pnorm a1 a2 b1 b2 Na Nb` where inorm=1,2,3 indicates a plane perpendiculer to x,y,z respectively. Within this plane (a1,b1) is the starting coordinate and (a2,b2) is the end coordinate. Na and Nb are the number of intervals along each direction. If inorm=1, a=y, b=z; if inorm=2, a=x, b=z; if inorm=3, a=x, b=y.

surfint Integrate over a specified surface giving $\int(expression)\mathrm{d}S$. The parameters are `ifrom ito` such that the surface exists between regions `ifrom` and `ito`. (the same concept as for Neuman boundaries, Section 3.3). The unit normal is available under variables `nx,ny,nz` and points from `ifrom` to `ito`. Derivative quantities may be used and are taken in the `ito` region evaluated on the surface.

volint Integrate over a volume within the region specified giving $\int(expression)\mathrm{d}V$. The single parameter is `region`, the region number to integrate over.

All calculations put their results into `.out` files named after the simulation with a numerical subscript. Thus, `file01.out, file02.out` etc. Linescans and planescans produce data which can be plotted in the form of a graph and indeed these graphs will be generated, in the form of EPS of EMF picture files, if `key_plot=1,2`. The integration commands simply output the integral result in their output files and no picture is generated. The interactive version of Zpp allows the user to view the graphs generated immediately but in any case the graphs are written to the simulation directory for the user to examine.

6.2 Scan expressions

Scan expressions basically have the same form as non-linear expressions Section 5.3. Expressions can depend on solved-for variables, the spatial position, the unit normal (surface intregration only), and constants in the `.con` file, see Table 5.1.

However, it is also possible to use *region dependent* expressions of the form

```
{reg1=expr1, reg2=expr2,...}
```

Here, `reg1` etc is a valid region number, `expr1` is the corresponding expression in the usual form Section 5.3. Note that *region expressions may not be nested*. Region expressions are introduced because different regions have different material properties and it is often necessary to chose the right one. An expression should be provided for each region traversed during the scan, or an error will result. For example, to calculate the x-component of the displacement field in the electrostatic calculation shown in Figure 5.5, we could use

```
linescan [parameters] = -{1=eps1,2=eps2}*Vx
```

In region 1, the expression evaluates to `-eps1*Vx`; in region 2, it becomes `-eps2*Vx`.

NOTE: Zpp reads the files `filename.con, filename.zin` so is aware of the constants specified e.g.,(`eps1,eps2`) and the variable names, e.g., (`V`).

Alternatively, the user may refer to the function `scanfun` in `filename.dll`. In this case, we use tokens beginning with $, eg

```
linescan [parameters] = $D

:


function scanfun(label,x,y,z,ur,dur,nvar)
  character(*) label
  integer nvar
  double precision scanfun,x,y,z,ur(nvar),dur(nvar,3)

  double precision, parameter :: eps0=8.854e-12
  double precision, parameter :: eps1=eps0,eps2=eps0*2
  double precision eps

  if (z.gt.0) then
    eps=eps1
  else
    eps=eps2
  endif

  scanfun=-eps*dur(1,1)
end function scanfun
```

would also generate the D-field. In this example, we assume that region 1 $z > 0$ and region 2 $z < 0$.

6.3 Example calculations

Let us assume an electrostatic calculation with V as the only variable (defined using the `labels` command in `.zin`). In that case

```
linescan 100    0.101 -0.3  -1.0     0.101 -0.3  +1.0 = V
```

creates a line scan graph of voltage from (0.101,-0.3,-1.0) to (0.101,-0.3,+1.0) with 100 points sampled.

```
linescan 100    0.101 -0.3  -1.0     0.101 -0.3  +1.0 = (V+1)^2/L
```

creates the same graph but plotting $(V+1)^2/L$ assuming constant L is defined in the `file.con` file.

```
linescan 100    0.101 -0.3  -1.0     0.101 -0.3  +1.0 = -Vz
```

creates a plot of $-\partial V/\partial z$ which is the z component of electric field (in this example).

```
  planescan      2  0.0   -1.0    1.0    -1.0    1.0    40  40 = &
-{1=eps1,2=eps2}*Vz
```

creates a planescan in the plane $y = 0.0$ with $x = [-1, 1]$ and $z = [-1, 1]$. A 40×40 grid will be generated. The expression is equal to `-eps1 Vz` in region 1 and `-eps2 Vz` in region 2. Recalling that Vz is $\partial V/dz$ and assuming the constants `eps1` and `eps2` are the permittivities of regions 1 and 2, the expression is the z component of electric displacement field (D-field).

```
surfint 2 1 = eps0*(Vx*nx+Vy*ny+Vz*nz)
```

Integrates over the surface between regions 1 and 2 and calculates

$$\int \epsilon_0 \mathbf{E} \cdot \mathbf{n} \, \mathrm{d}S \tag{6.1}$$

In this case the electric field is evaluated on the region 1 side of the interface (the second region specified) and the unit normal points *from* region 2 *to* region 1. If region 1 is vacuum and region 2 is a fixed potential electrode region, this integral will give the electric charge on the electrode.

6.4 Zpp output files

filename01.out, filename02.out,.. Output files corresponding to the scans in `filename.zpp` in the order they were defined. In the transient case, all specified snapshots are output in each file, each separated by a double blank line. These files can be plotted with any graph plotter or spreadsheet. The timestep for each snapshot is indicaed in the file.

filename01.eps, filename02.eps,.. In the case, `key_plot=1`, these are graphs are generated by gnuplot corresponding to the scans requested.

filename01.emf, filename02.emf,.. In the case, `key_plot=2`, these are graphs are generated by gnuplot corresponding to the scans requested.

Bibliography

[1] Field Precision Ltd, PO Box 13595, Albuquerque, New Mexico 87192 USA, www.fieldp.com

[2] MetaMesh, Three-dimensional Conformal Mesh generator, Field Precision (2003).

[3] ASEN 5367 – Advanced Finite Element Methods, Carlos A. Felippa, Aerospace Engineering Sciences, University of Colorado at Boulder, www.colorado.edu, (2006), Chapter 18

Appendix A

Comsol's coefficient mode

Comsol allows the user to specify PDEs in the form

$$\nabla \cdot (-\mathbf{C}\nabla\mathbf{u} - \boldsymbol{\alpha}\mathbf{u} + \boldsymbol{\gamma}) + \mathbf{a}\mathbf{u} + \boldsymbol{\beta} \cdot \nabla\mathbf{u} = \mathbf{f} \tag{A.1}$$

$$\mathbf{n} \cdot (\mathbf{C}\nabla\mathbf{u} + \boldsymbol{\alpha}\mathbf{u} - \boldsymbol{\gamma}) + \mathbf{q}\mathbf{u} = \mathbf{g} - \mathbf{h}^T\boldsymbol{\mu}, \quad \text{(Neumann)} \tag{A.2}$$

$$\mathbf{h}\mathbf{u} = \mathbf{r}, \quad \text{(Dirichlet)} \tag{A.3}$$

Here $\mathbf{u} = (u_1, u_2, ...)$ where $u_1(x, y, z)$ etc are the independent variables to be solved for. For example u_1 might be electrostatic potential and u_2 temperature as in Section 4.4. One must set the various components of C etc so that, when (A.1) is multiplied out, we obtain the needed set of PDEs. Here, the meaning of grad and div is non-standard. For example, with two variables, we define

$$\nabla\mathbf{u} = (\nabla u_1, \nabla u_2) \tag{A.4}$$

$$\nabla \cdot (\mathbf{a}|\mathbf{b}) = (\nabla \cdot \mathbf{a}, \nabla \cdot \mathbf{b}) \tag{A.5}$$

where $(\mathbf{a}|\mathbf{b})$ is a 6-vector (in 3D space) partitioned into two, 3-vectors.

In principle, ZINC could be extended to allow the other variables in (A.1). However, the boundary condition variables $\mathbf{q}$ and $\mathbf{g}$ would be difficult to do in ZINC as these require a surface integral to be added to the energy function. Currently the mesh specification file `zinc.mtf` does not identify mesh faces so this would not be possible.

Note that comsol uses a Lagrange multiplier $\boldsymbol{\mu}$. This means that when Dirichlet boundary conditions are used, the Neumann equation (A.2) becomes trivial. When Dirichlet is not set (so that $\mathbf{h} = 0$) we default to the Neumann boundary.

Appendix B

Description of the zinc.mtf file

Consider the illustration Figure B.1. Here the problem is shown in 2-D for clarity. The 3-D mesh used in ZINCis analogous. In the figure, there are 3 material regions and we need to label the elements as region 1, 2 or 3 appropriately (we will later associate material properties with each region). We want to label the top row of nodes as region 4 and the bottom row as region 5. (We will later set Dirichlet boundaries for nodes with region number 4 and 5). The region numbers of the internal nodes does not matter provided it is not 4 or 5. Nodes with numbers 1, 2 or 3 will not be fixed. We will label internal nodes as 1. Note: Metamesh will generally label the internal nodes the same as adjacent elements as it performs the mesh.

Nodes are indexed as (0,0), (1,0) etc. Node (2,1) is indicated in the figure. The complete zinc.mtf file would be:

```
IMax:  3
JMax:  3

 I    J    x    y    RegNo   RegUp
==================================
 0    0   0.0  0.0       5       3
 1    0   0.5  0.0       5       3
 2    0   etc...         5       3
 3    0                  5       0
 0    1                  1       2
 1    1                  1       2
 2    1                  1       2
 3    1                  1       0
 0    2                  1       1
 1    2                  1       1
 2    2                  1       1
 3    2                  1       0
 0    3                  4       0
 1    3                  4       0
 2    3                  4       0
 3    3                  4       0
```

RegNo specifies the region number of the node in question. RegUp specified the region number

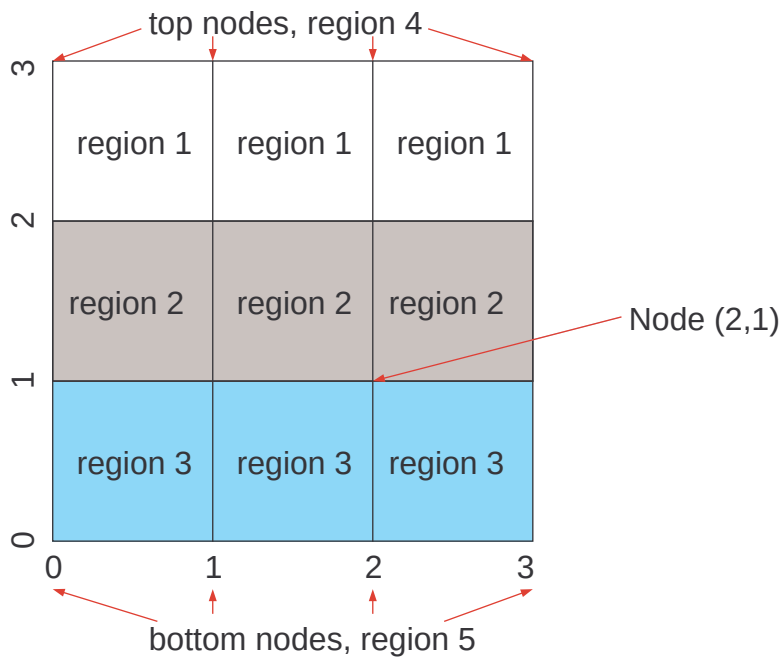


Figure B.1: 2-D analogue of ZINCmeshing.

of the element connected to this node in the positive I, J (and K for the 3-D case) direction. Note that elements which do not exists are labelled "0".

Assuming one variable, the corresponding `filename.zin` file would be something like

```
region 1 elements 3 values C
1 1 1 1   2e-6
1 2 1 2   2e-6
1 3 1 3   2e-6

region 2 elements 4 values C
1 1 1 1   7e-6
1 1 1 2   4e-6
1 2 1 2   7e-6
1 3 1 3   7e-6

region 3 elements 6 values C
1 1 1 1   4e-6
1 2 1 2   4e-6
1 3 1 3   4e-6
1 1 1 2   3.6e-6
1 1 1 3   3.2e-6
1 3 1 3   7e-6
```

```
region 4 nodes 1 value
1 1.0

region 5 nodes 1 value
1 2.0
```

Appendix C

Additional global variables in file.zin

These options should only be used by developers or if you are feeling adventurous!

key_db 0: no debug info; 1: write debug info to `zinc.out`; 2: write detailed debug information. Create files showing shape of each element. (default 0)

idmin, idbmax, jdbmin, jdbmax, kdbmin, kdbmax range for elements (specified by lower nodes) to be written for debuging. Only used when key db=2

key_Q 1: Build Q by node pairs (seems to be faster); 2 build Q by element (does not implement Surface commands). (default 1)